Non Target Peaks Area Percent Report

Data Path : C:\msdchem\1\LEGACY\2012\January\
Data File : 011012PA-[redacted]8-Day1.D
Acq On : 10 Jan 2012 9:40
Operator :
Sample : PA-[redacted]8-Day1
Misc : 1.0 uL PA-[redacted]8-Day1 at 1 mL
ALS Vial : 54 Sample Multiplier: 1

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : C:\msdchem\1\METHODS\TLTICPAH.M
Title : PAH5437

Signal : TIC: 011012PA-[redacted]8-Day1.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	9.598	417	431	454	rBV	10014780	29177393	9.01%	3.752%
2	9.807	458	476	517	rVB	2645587	14054121	4.34%	1.807%
3	12.410	1027	1035	1063	rBV	6808847	19286111	5.96%	2.480%
4	12.629	1074	1082	1093	rBV	5166008	11156330	3.45%	1.435%
5	13.201	1198	1205	1217	rVV4	3058039	10769844	3.33%	1.385%
6	13.369	1234	1241	1253	rVV2	5256978	11712202	3.62%	1.506%
7	13.499	1255	1269	1282	rVB2	12070192	33209937	10.26%	4.271%
8	13.890	1345	1353	1361	rVB	14034858	26075256	8.06%	3.353%
9	14.146	1402	1408	1415	rVB	5075003	10081026	3.11%	1.296%
10	14.556	1487	1496	1501	rBV2	6455039	14924810	4.61%	1.919%
11	14.793	1539	1547	1561	rBV2	8367968	24778602	7.65%	3.186%
12	14.896	1562	1569	1580	rVB	6269358	14519395	4.49%	1.867%
13	14.989	1580	1589	1597	rBV	17001498	32768881	10.12%	4.214%
14	15.319	1653	1660	1667	rBV	9692034	18658068	5.76%	2.399%
15	15.878	1774	1780	1796	rVB2	4140599	9759129	3.01%	1.255%
16	16.087	1820	1825	1837	rVB3	6604896	14165692	4.38%	1.822%
17	16.250	1850	1860	1879	rVV2	15381914	38865889	12.01%	4.998%
18	18.336	2244	2308	2321	rBV2	32453500	323695728	100.00%	41.626%
19	25.547	3840	3857	3875	rVB	5012409	17099757	5.28%	2.199%
20	29.001	4577	4599	4712	rVB8	841329	11878230	3.67%	1.527%
21	33.773	5594	5624	5743	rBV9	813573	14624431	4.52%	1.881%
22	37.148	6316	6349	6484	rBV3	1858327	40455957	12.50%	5.202%
23	39.075	6728	6763	6899	rBV8	743577	15794734	4.88%	2.031%
24	42.660	7495	7533	7540	rBV7	2203802	20115808	6.21%	2.587%

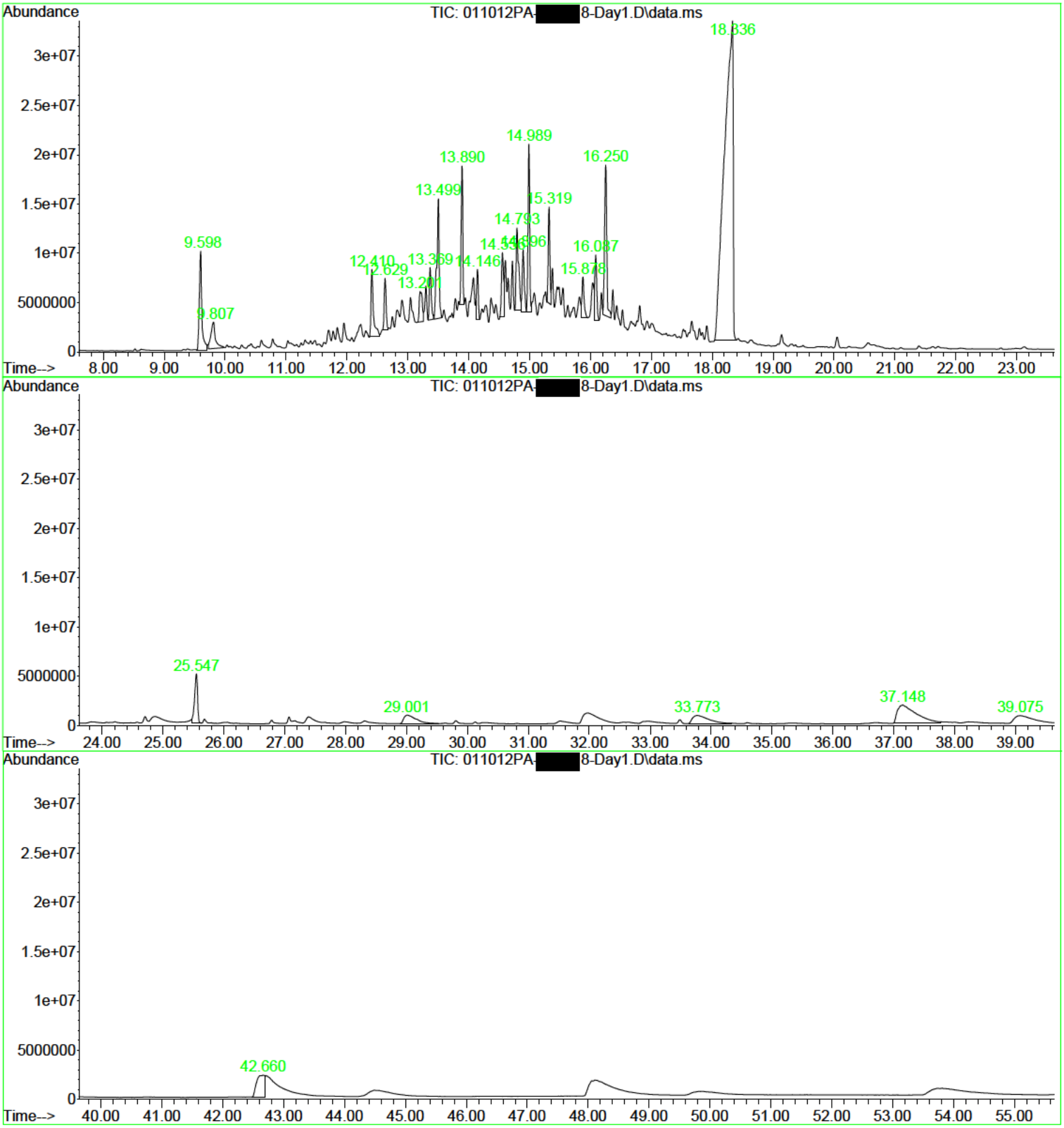
Sum of corrected areas: 777627331

Non Target Peaks Report - Integrated Chromatogram

Data Path : C:\msdchem\1\LEGACY\2012\January\
Data File : 011012PA-[redacted]8-Day1.D
Acq On : 10 Jan 2012 9:40
Operator :
Sample : PA-[redacted]8-Day1
Misc : 1.0 uL PA-[redacted]8-Day1 at 1 mL
ALS Vial : 54 Sample Multiplier: 1

Quant Method : C:\msdchem\1\METHODS\TLTICPAH.M
Quant Title : PAH5437

TIC Library : C:\Database\NIST08.L
TIC Integration Parameters: rteint.p



Non Target Peak Search Report

Data Path : C:\msdchem\1\LEGACY\2012\January\
Data File : 011012PA-[redacted]8-Day1.D
Acq On : 10 Jan 2012 9:40
Operator :
Sample : PA-Blaker8-Day1
Misc : 1.0 uL PA-[redacted]8-Day1 at 1 mL
ALS Vial : 54 Sample Multiplier: 1

Quant Method : C:\msdchem\1\METHODS\TLTICPAH.M
Quant Title : PAH5437

TIC Library : C:\Database\NIST08.L
TIC Integration Parameters: rteint.p

****

Peak Number 1 Tetramethylbutanedinitrile Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.598	2917.74 ng	29177400	External Standard	0.000

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetramethylbutanedinitrile	136	C8H12N2	003333-52-6	83
2	Propanenitrile, 2,2'-azobis[2-me...	164	C8H12N4	000078-67-1	83
3	Tetramethylbutanedinitrile	136	C8H12N2	003333-52-6	83
4	1,5-Pentanediol, o,o'-di(proparg...	268	C13H16O6	1000331-35-4	45
5	Propanenitrile, 2,2'-azobis[2-me...	164	C8H12N4	000078-67-1	35

****

Peak Number 2 Formamide, N-methylthio Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.807	1405.41 ng	14054100	External Standard	0.000

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Formamide, N-methylthio	75	C2H5NS	018952-41-5	78
2	Ethanethioamide	75	C2H5NS	000062-55-5	5
3	Ethanethioamide	75	C2H5NS	000062-55-5	5
4	o-Isopropylhydroxylamine	75	C3H9NO	1000322-42-6	4
5	Formamide, N-methoxy-	75	C2H5NO2	034005-41-9	4

****

Peak Number 3 Dodecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.410	1928.61 ng	19286100	External Standard	0.000

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	95
2	Dodecane	170	C12H26	000112-40-3	94
3	Dodecane	170	C12H26	000112-40-3	90
4	Tetradecane	198	C14H30	000629-59-4	86
5	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	80

****

Peak Number 4 Dodecane, 2-methyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.369	1171.22 ng	11712200	External Standard	0.000

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-	184	C13H28	001560-97-0	93
2	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	72
3	Undecane, 3-methyl-	170	C12H26	001002-43-3	72

Data Path : C:\msdchem\1\LEGACY\2012\January\
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Acq On : 10 Jan 2012 9:40
Operator :
Sample : PA-Blaker8-Day1
Misc : 1.0 uL PA-[redacted]8-Day1 at 1 mL
ALS Vial : 54 Sample Multiplier: 1

Quant Method : C:\msdchem\1\METHODS\TLTICPAH.M
Quant Title : PAH5437

TIC Library : C:\Database\NIST08.L
TIC Integration Parameters: rteint.p

4	Dodecane, 2-methyl-	184	C13H28	001560-97-0	64
5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	59

****

Peak Number 5 Octane, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.499	3320.99 ng	33209900	External Standard	0.000

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	87
2	Nonane, 3-methyl-	142	C10H22	005911-04-6	83
3	Bacchotricuneatin c	342	C20H22O5	066563-30-2	72
4	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	72
5	Decane, 4-methyl-	156	C11H24	002847-72-5	64

****

Peak Number 6 Tridecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.890	2607.53 ng	26075300	External Standard	0.000

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	97
2	Tridecane	184	C13H28	000629-50-5	97
3	Tridecane	184	C13H28	000629-50-5	93
4	Tridecane	184	C13H28	000629-50-5	90
5	Hexadecane	226	C16H34	000544-76-3	90

****

Peak Number 7 Heptylcyclohexane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.556	1492.48 ng	14924800	External Standard	0.000

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptylcyclohexane	182	C13H26	005617-41-4	90
2	Cyclohexane, undecyl-	238	C17H34	054105-66-7	86
3	Cyclohexane, (4-methylpentyl)-	168	C12H24	061142-20-9	80
4	Cyclohexane, hexyl-	168	C12H24	004292-75-5	72
5	Heptylcyclohexane	182	C13H26	005617-41-4	68

****

Peak Number 8 Tridecane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.793	2477.86 ng	24778600	External Standard	0.000

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual

Non Target Peak Search Report

Data Path : C:\msdchem\1\LEGACY\2012\January\
Data File : 011012PA-[redacted]8-Day1.D
Acq On : 10 Jan 2012 9:40
Operator :
Sample : PA[redacted]8-Day1
Misc : 1.0 uL PA-[redacted]8-Day1 at 1 mL
ALS Vial : 54 Sample Multiplier: 1

Quant Method : C:\msdchem\1\METHODS\TLTICPAH.M
Quant Title : PAH5437

TIC Library : C:\Database\NIST08.L
TIC Integration Parameters: rteint.p

1	Tridecane, 2-methyl-	198	C14H30	001560-96-9 93
2	Tridecane, 2-methyl-	198	C14H30	001560-96-9 83
3	Tridecane, 2-methyl-	198	C14H30	001560-96-9 81
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7 80
5	Heptadecane	240	C17H36	000629-78-7 80

****
Peak Number 9 3,5-Dimethyldodecane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.896	1451.94 ng	14519400	External Standard	0.000

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Dimethyldodecane	198	C14H30	107770-99-0	83
2	2,6-Dimethyldecane	170	C12H26	013150-81-7	76
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	72
4	Dodecane, 2-methyl-	184	C13H28	001560-97-0	53
5	Octacosane	394	C28H58	000630-02-4	53

****
Peak Number 10 Hexadecane, 2,6,10,14-tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.989	3276.89 ng	32768900	External Standard	0.000

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	90
2	Decane, 5-propyl-	184	C13H28	017312-62-8	72
3	Tetradecane, 4-methyl-	212	C15H32	025117-24-2	72
4	Bacchotricuneatin c	342	C20H22O5	066563-30-2	64
5	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	64

****
Peak Number 11 Tetradecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.319	1865.81 ng	18658100	External Standard	0.000

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	96
2	Tetradecane	198	C14H30	000629-59-4	96
3	Tetradecane	198	C14H30	000629-59-4	95
4	Octadecane	254	C18H38	000593-45-3	93
5	Tetradecane	198	C14H30	000629-59-4	93

****
Peak Number 12 Cyclohexane, octyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.

Data Path : C:\msdchem\1\LEGACY\2012\January\
Data File : 011012PA-[redacted]8-Day1.D
Acq On : 10 Jan 2012 9:40
Operator :
Sample : PA-[redacted]8-Day1
Misc : 1.0 uL PA-[redacted]8-Day1 at 1 mL
ALS Vial : 54 Sample Multiplier: 1

Quant Method : C:\msdchem\1\METHODS\TLTICPAH.M
Quant Title : PAH5437

TIC Library : C:\Database\NIST08.L
TIC Integration Parameters: rteint.p

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.087	1416.57 ng	14165700	External Standard	0.000

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, octyl-	196	C14H28	001795-15-9	68
2	Cyclohexane, pentyl-	154	C11H22	004292-92-6	59
3	Cyclohexane, (4-methylpentyl)-	168	C12H24	061142-20-9	59
4	Cyclohexane, octyl-	196	C14H28	001795-15-9	59
5	Cyclohexane, pentyl-	154	C11H22	004292-92-6	59

****

Peak Number 13 Hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.250	3886.59 ng	38865900	External Standard	0.000

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	93
2	Bacchotricuneatin c	342	C20H22O5	066563-30-2	92
3	Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	90
4	Pentadecane, 4-methyl-	226	C16H34	002801-87-8	81
5	Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	81

****

Peak Number 14 Hexahydro-1,3,5-trimethyl-1... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.336	32369.60 ng	323696000	External Standard	0.000

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexahydro-1,3,5-trimethyl-1,3,5-...	159	C6H13N3S	059887-80-8	72
2	Quinoline, 6-methoxy-	159	C10H9NO	005263-87-6	50
3	8-Quinolinol, 4-methyl-	159	C10H9NO	003846-73-9	37
4	Oxazole, 4-methyl-2-phenyl-	159	C10H9NO	000877-39-4	25
5	4,6-Difluoro-2-dimethylaminopyri...	159	C6H7F2N3	165258-63-9	9

****

Peak Number 15 Cyclic octaatomic sulfur Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.547	1709.98 ng	17099800	External Standard	0.000

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclic octaatomic sulfur	256	S8	010544-50-0	52
2	Benzoic acid, 2,5-dinitro-	212	C7H4N2O6	000610-28-6	32
3	7-Amino-7H-S-triazolo[5,1-c]-S-t...	156	C3H4N6S	013728-28-4	28
4	N,N'-Pentamethylenebis[s-3-amino...	410	C11H26N2O6S4	035871-54-6	25
5	Benzofuran, 3-(4-chlorophenyl)-2...	256	C16H13ClO	074228-99-2	9

Non Target Peak Search Report

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Data File : 011012PA-[redacted]8-Day1.D
Acq On : 10 Jan 2012 9:40
Operator :
Sample : PA-Blaker8-Day1
Misc : 1.0 uL PA-[redacted]8-Day1 at 1 mL
ALS Vial : 54 Sample Multiplier: 1

Quant Method : C:\msdchem\1\METHODS\TLTICPAH.M
Quant Title : PAH5437

TIC Library : C:\Database\NIST08.L
TIC Integration Parameters: rteint.p

****
Peak Number 16 Butyric acid, octadecyl ester Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.001	1187.82 ng	11878200	External Standard	0.000

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyric acid, octadecyl ester	340	C22H44O2	013373-83-6	64
2	Tetraethylene glycol monododecyl...	362	C20H42O5	005274-68-0	64
3	Isobutyric acid, octadecyl ester	340	C22H44O2	013373-82-5	59
4	3-(2,5,8,11,14-Pentaoxacyclohexa...	510	C24H46O11	1000110-99-4	59
5	3-Hydroxymyristic acid	244	C14H28O3	001961-72-4	53

****
Peak Number 17 Heptaethylene glycol monodo... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
33.773	1462.44 ng	14624400	External Standard	0.000

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptaethylene glycol monododecyl...	494	C26H54O8	003055-97-8	86
2	Pentaethylene glycol monododecyl...	406	C22H46O6	003055-95-6	86
3	Pentaethylene glycol	238	C10H22O6	004792-15-8	86
4	Tetraethylene glycol monododecyl...	362	C20H42O5	005274-68-0	83
5	Hexagol	282	C12H26O7	002615-15-8	72

****
Peak Number 18 Bis(dibutylamino)dichlorosi... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
37.148	4045.60 ng	40456000	External Standard	0.000

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bis(dibutylamino)dichlorosilane	354	C16H36Cl2N2Si	1000322-56-4	43
2	Naphthalen-1-amine, N-(5-methoxy...	311	C22H17NO	1000276-25-8	28
3	Quinazolin-4(3H)-one, 3-(4-metho...	311	C16H13N3O4	1000268-92-7	25
4	Ethanol, 2-[2-[2-[2-[p-(1,1,3,3-...	382	C22H38O5	002315-63-1	16
5	3,6,9,12,15-Pentaoxabicyclo[15.3...	312	C16H24O6	065112-36-9	10

****
Peak Number 19 Hexagol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
39.075	1579.47 ng	15794700	External Standard	0.000

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexagol	282	C12H26O7	002615-15-8	86
2	Hexagol	282	C12H26O7	002615-15-8	86
3	2-[2-[2-[2-[2-[2-(2-Hydroxyethox...	326	C14H30O8	1000352-13-3	80

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Misc : 1.0 uL PA-[redacted]8-Day1 at 1 mL
ALS Vial : 54 Sample Multiplier: 1

Quant Method : C:\msdchem\1\METHODS\TLTICPAH.M
Quant Title : PAH5437

TIC Library : C:\Database\NIST08.L
TIC Integration Parameters: rteint.p

4	Octaethylene glycol	370	C16H34O9	1000289-34-2 80
5	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1 80

****

Peak Number 20 Cobalt, bis(.eta.-5-piperid... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
42.660	2011.58 ng	20115800	External Standard	0.000

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cobalt, bis(.eta.-5-piperidinylc...	355	C20H28CoN2	1000162-04-6	27
2	Aspidospermidine-1-ethanol, 17-h...	386	C23H34N2O3	054725-07-4	27
3	Silane, dimethyl(4-(2-phenylprop...	370	C23H34O2Si	1000347-19-1	12
4	1,2-Dihydro-2-methylpapaverine	355	C21H25NO4	1000128-57-7	12
5	(4-Methyl-6-phenylpyrimidin-2-yl...	355	C22H21N5	1000303-17-5	12

Non Target Peaks Summary

Data Path : C:\msdchem\1\LEGACY\2012\January\
Data File : 011012PA-[redacted]8-Day1.D
Acq On : 10 Jan 2012 9:40
Operator :
Sample : PA-Blaker8-Day1
Misc : 1.0 uL PA-[redacted]8-Day1 at 1 mL
ALS Vial : 54 Sample Multiplier: 1

Quant Method : C:\msdchem\1\METHODS\TLTICPAH.M
Quant Title : PAH5437

TIC Library : C:\Database\NIST08.L
TIC Integration Parameters: rteint.p

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Tetramethylbuta...	9.598	2917.7	ng	29177400	0	0.000	10000	1.0
Formamide, N-me...	9.807	1405.4	ng	14054100	0	0.000	10000	1.0
Dodecane	12.410	1928.6	ng	19286100	0	0.000	10000	1.0
Dodecane, 2-met...	13.369	1171.2	ng	11712200	0	0.000	10000	1.0
Octane, 2,6-dim...	13.499	3321.0	ng	33209900	0	0.000	10000	1.0
Tridecane	13.890	2607.5	ng	26075300	0	0.000	10000	1.0
Heptylcyclohexane	14.556	1492.5	ng	14924800	0	0.000	10000	1.0
Tridecane, 2-me...	14.793	2477.9	ng	24778600	0	0.000	10000	1.0
3,5-Dimethyldod...	14.896	1451.9	ng	14519400	0	0.000	10000	1.0
Hexadecane, 2,6...	14.989	3276.9	ng	32768900	0	0.000	10000	1.0
Tetradecane	15.319	1865.8	ng	18658100	0	0.000	10000	1.0
Cyclohexane, oc...	16.087	1416.6	ng	14165700	0	0.000	10000	1.0
Hexadecane	16.250	3886.6	ng	38865900	0	0.000	10000	1.0
Hexahydro-1,3,5...	18.336	32369.6	ng	323696000	0	0.000	10000	1.0
Cyclic octaatom...	25.547	1710.0	ng	17099800	0	0.000	10000	1.0
Butyric acid, o...	29.001	1187.8	ng	11878200	0	0.000	10000	1.0
Heptaethylene g...	33.773	1462.4	ng	14624400	0	0.000	10000	1.0
Bis(dibutylamin...	37.148	4045.6	ng	40456000	0	0.000	10000	1.0
Hexagol	39.075	1579.5	ng	15794700	0	0.000	10000	1.0
Cobalt, bis(.et...	42.660	2011.6	ng	20115800	0	0.000	10000	1.0