LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
Data File : BF109058.D
Acq On : 17 Sep 2018 19:46
Operator : JU/SJ
Sample : J4946-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RB12983RT

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 : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.901	433	436	443	rVB	51198	58592	4.37%	0.341%
2	5.325	504	508	512	rBV	1519131	1341460	100.00%	7.816%
3	6.354	678	683	691	rBV	1413739	1334696	99.50%	7.777%
4	6.489	702	706	709	rBV	1542433	1341431	100.00%	7.816%
5	6.719	742	745	749	rBV	761237	640592	47.75%	3.732%
6	6.878	768	772	775	rBV	1229926	955629	71.24%	5.568%
7	7.125	810	814	821	rBV	20731	22812	1.70%	0.133%
8	7.278	836	840	843	rBV	915417	746679	55.66%	4.351%
9	8.001	959	963	966	rBV	892692	707685	52.75%	4.123%
10	8.030	966	968	971	rVB2	22847	18419	1.37%	0.107%
11	9.036	1136	1139	1142	rVB	19548	17785	1.33%	0.104%
12	9.077	1142	1146	1149	rBV	1317712	1030566	76.82%	6.005%
13	9.172	1156	1162	1166	rBV5	27162	42926	3.20%	0.250%
14	9.395	1196	1200	1201	rBV2	28997	29470	2.20%	0.172%
15	9.425	1202	1205	1210	rVV	70812	81116	6.05%	0.473%
16	9.472	1210	1213	1215	rVV	185215	163681	12.20%	0.954%
17	9.495	1215	1217	1219	rVV2	52173	43684	3.26%	0.255%
18	9.524	1219	1222	1227	rVV7	13436	29123	2.17%	0.170%
19	9.636	1237	1241	1245	rBV4	26634	57850	4.31%	0.337%
20	9.672	1245	1247	1250	rVB	66184	52038	3.88%	0.303%
21	9.707	1250	1253	1255	rBV4	26104	37580	2.80%	0.219%
22	9.754	1256	1261	1265	rBV	840912	850753	63.42%	4.957%
23	10.024	1305	1307	1311	rBV3	67934	65755	4.90%	0.383%
24	10.166	1328	1331	1335	rBV4	74713	78266	5.83%	0.456%
25	10.295	1351	1353	1355	rBV2	49875	49103	3.66%	0.286%
26	10.419	1371	1374	1377	rVB	132361	130221	9.71%	0.759%
27	10.530	1390	1393	1398	rBV	882148	837185	62.41%	4.878%
28	10.683	1416	1419	1424	rVB	346727	350483	26.13%	2.042%
29	11.148	1495	1498	1502	rVB	572433	524345	39.09%	3.055%
30	11.230	1509	1512	1514	rBV	945931	753031	56.14%	4.388%
31	11.254	1514	1516	1519	rVB2	210131	176809	13.18%	1.030%
32	11.501	1555	1558	1560	rBV	144244	144859	10.80%	0.844%
33	12.436	1714	1717	1720	rBV	309762	289766	21.60%	1.688%
34	12.660	1753	1755	1758	rVB	227036	176715	13.17%	1.030%

LSC Area Percent Report

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Acq On : 17 Sep 2018 19:46
Operator : JU/SJ
Sample : J4946-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RB12983RT

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 : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.813	1777	1781	1787	rVB	1184945	1149955	85.72%	6.700%
36	13.718	1932	1935	1945	rVB2	139071	219384	16.35%	1.278%
37	13.854	1954	1958	1961	rBV	1189197	1149704	85.71%	6.699%
38	13.877	1961	1962	1965	rVB	129355	73882	5.51%	0.430%
39	14.707	2101	2103	2107	rVB	60452	55824	4.16%	0.325%
40	14.859	2126	2129	2132	rBV	75148	100764	7.51%	0.587%
41	14.954	2143	2145	2150	rVB2	75193	87261	6.50%	0.508%
42	15.142	2174	2177	2179	rBV	53483	55523	4.14%	0.324%
43	15.195	2183	2186	2192	rVV	140187	256556	19.13%	1.495%
44	15.254	2192	2196	2202	rVV	572420	715340	53.33%	4.168%
45	15.306	2203	2205	2210	rVB	53751	61544	4.59%	0.359%
46	15.712	2272	2274	2279	rVB2	45482	56093	4.18%	0.327%

Sum of corrected areas: 17162935

LSC Report - Integrated Chromatogram

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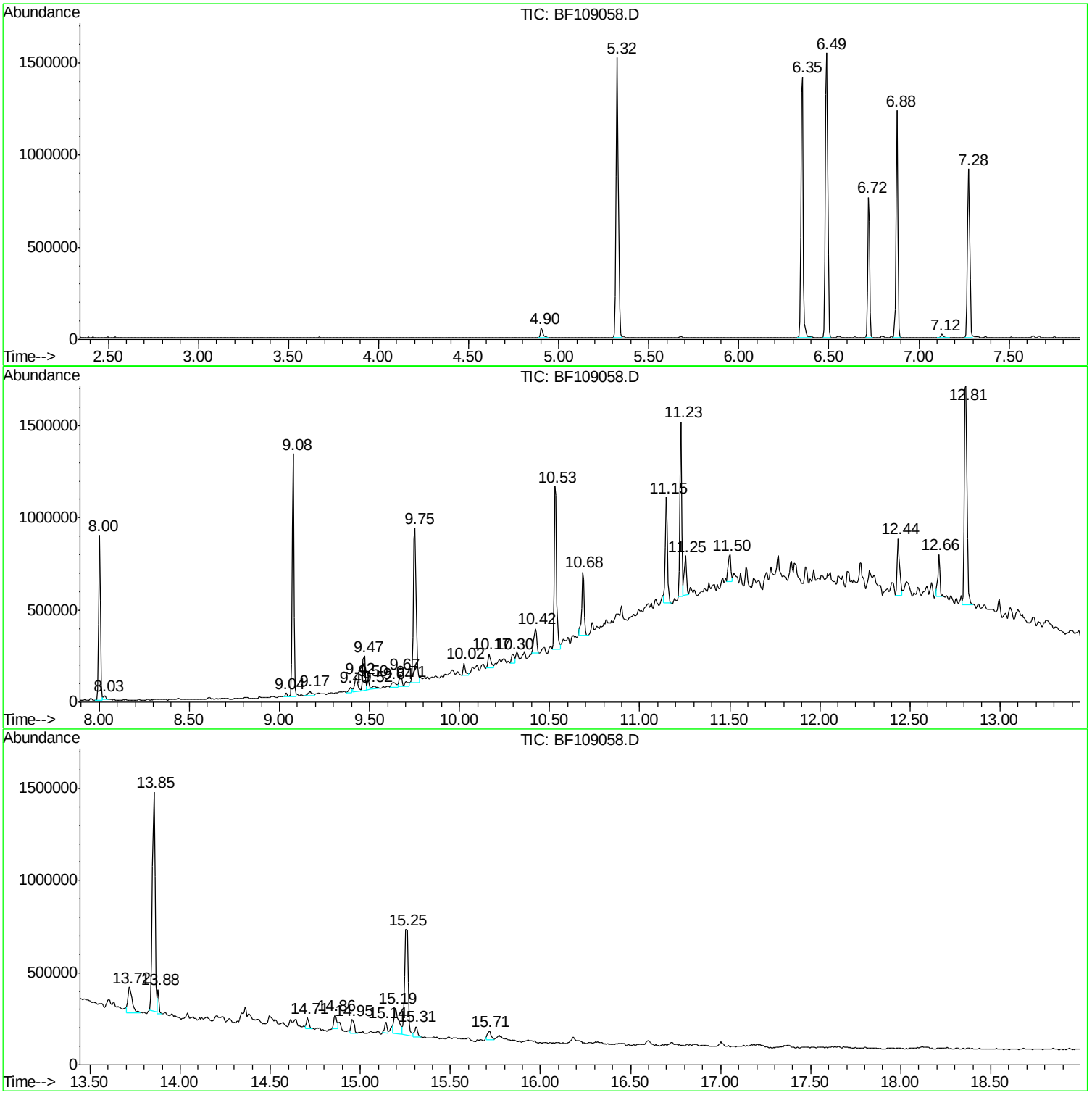
Operator : JU/SJ
Sample : J4946-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RB12983RT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
Data File : BF109058.D
Acq On : 17 Sep 2018 19:46
Operator : JU/SJ
Sample : J4946-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RB12983RT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

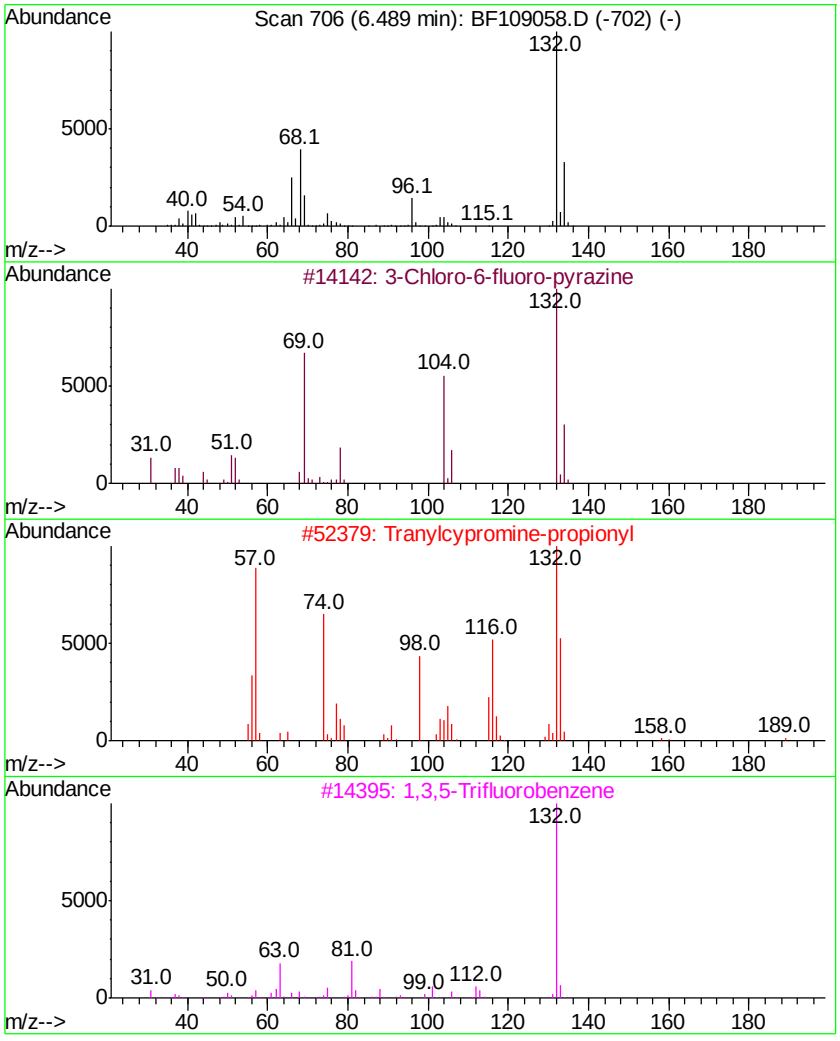
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

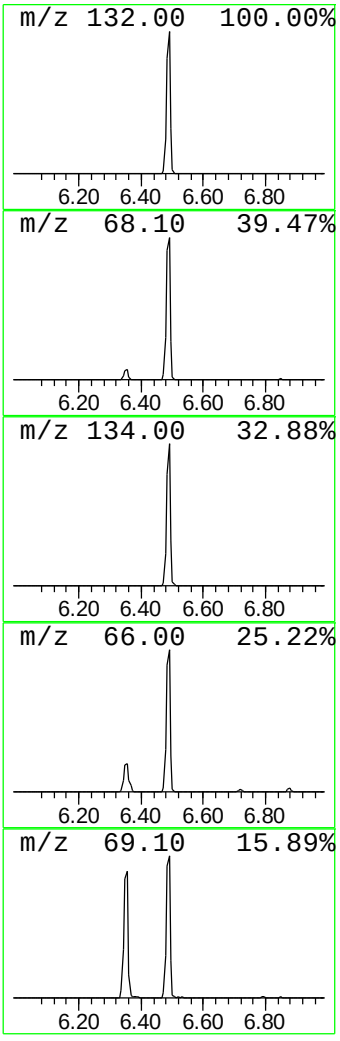
****

Peak Number 1 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	41.88 ng	1341430	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





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Data File : BF109058.D
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Operator : JU/SJ
Sample : J4946-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RB12983RT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

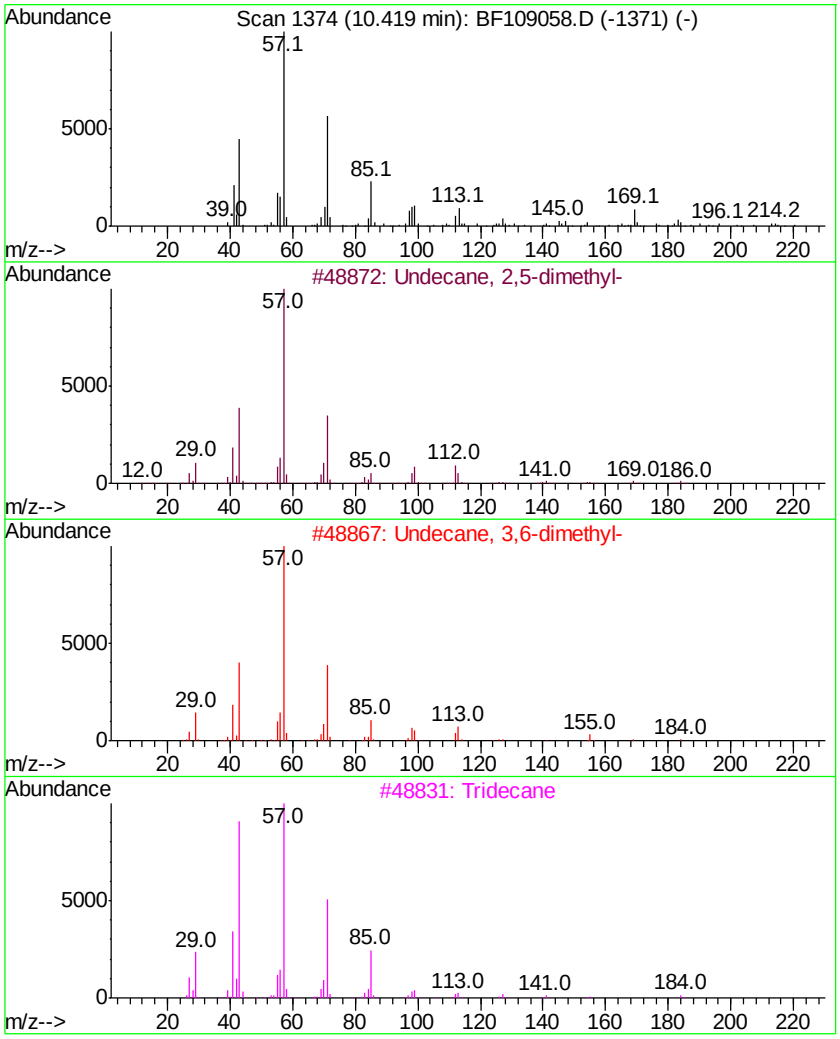
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

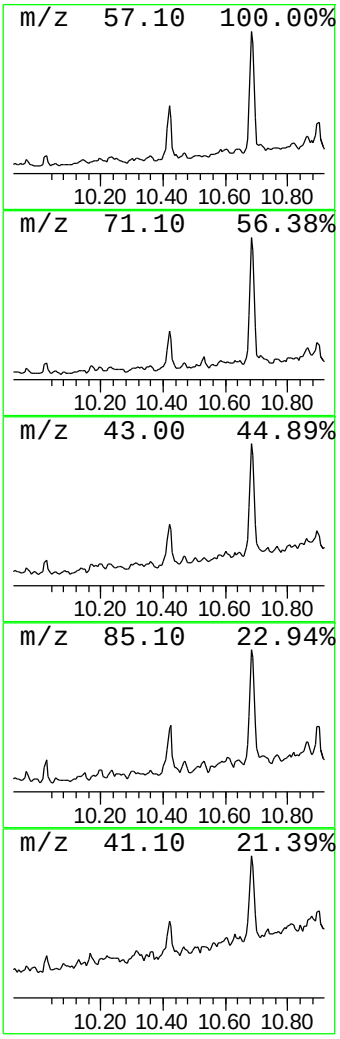
****

Peak Number 3 Undecane, 2,5-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.42	3.06 ng	130221	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	64
2	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	64
3	Tridecane	184	C13H28	000629-50-5	64
4	Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1000309-19-2	58
5	Sulfurous acid, pentyl tetradecy...	348	C19H40O3S	1000309-14-7	49





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
Data File : BF109058.D
Acq On : 17 Sep 2018 19:46
Operator : JU/SJ
Sample : J4946-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RB12983RT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

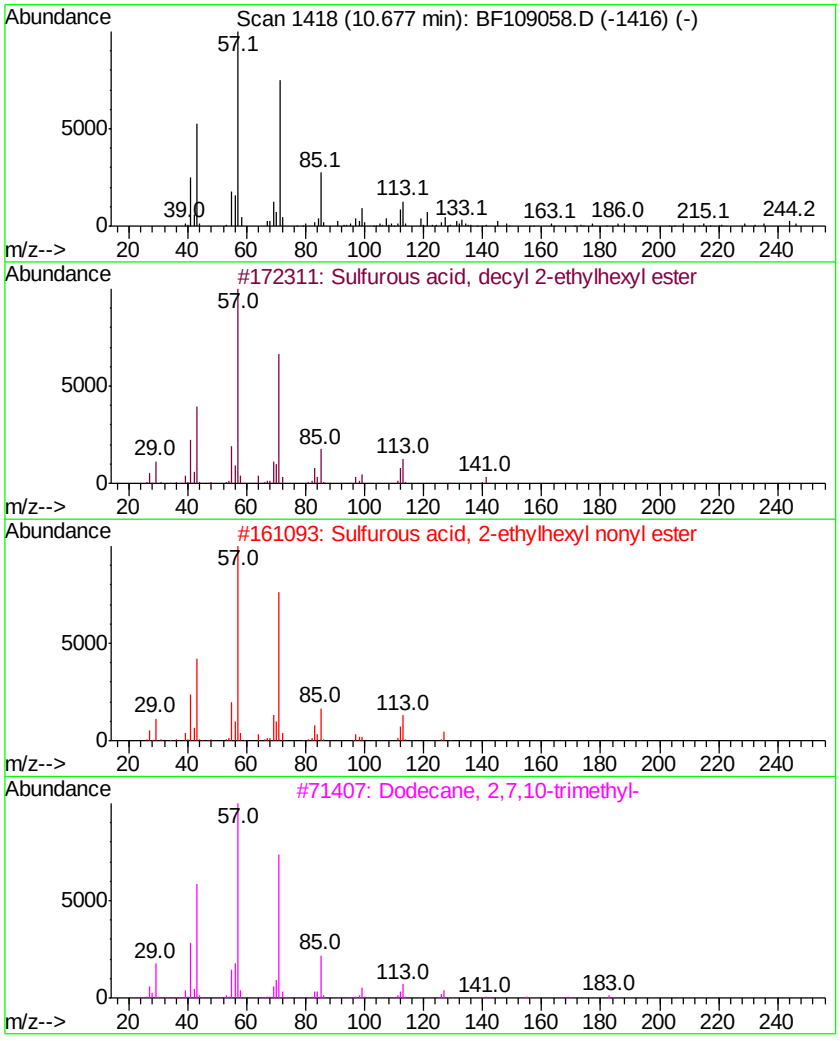
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

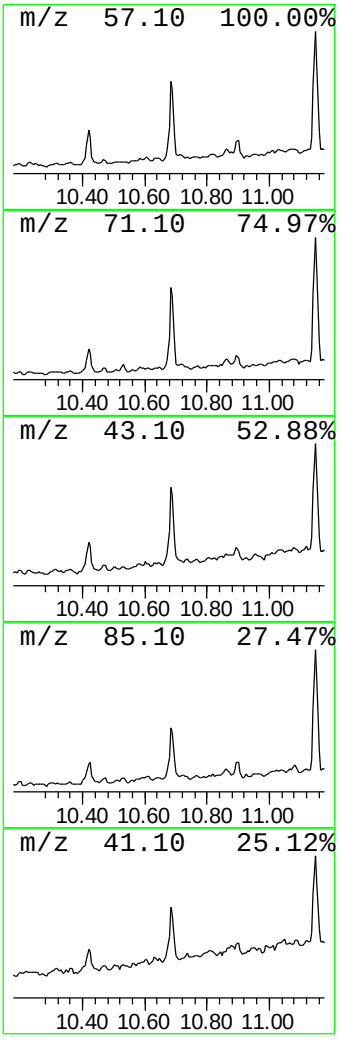
****

Peak Number 4 Sulfurous acid, decyl 2-eth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.68	9.31 ng	350483	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	80
2	Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1000309-19-2	72
3	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	72
4	Octadecane	254	C18H38	000593-45-3	59
5	Dodecane	170	C12H26	000112-40-3	59





Library Search Compound Report

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Sample : J4946-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RB12983RT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
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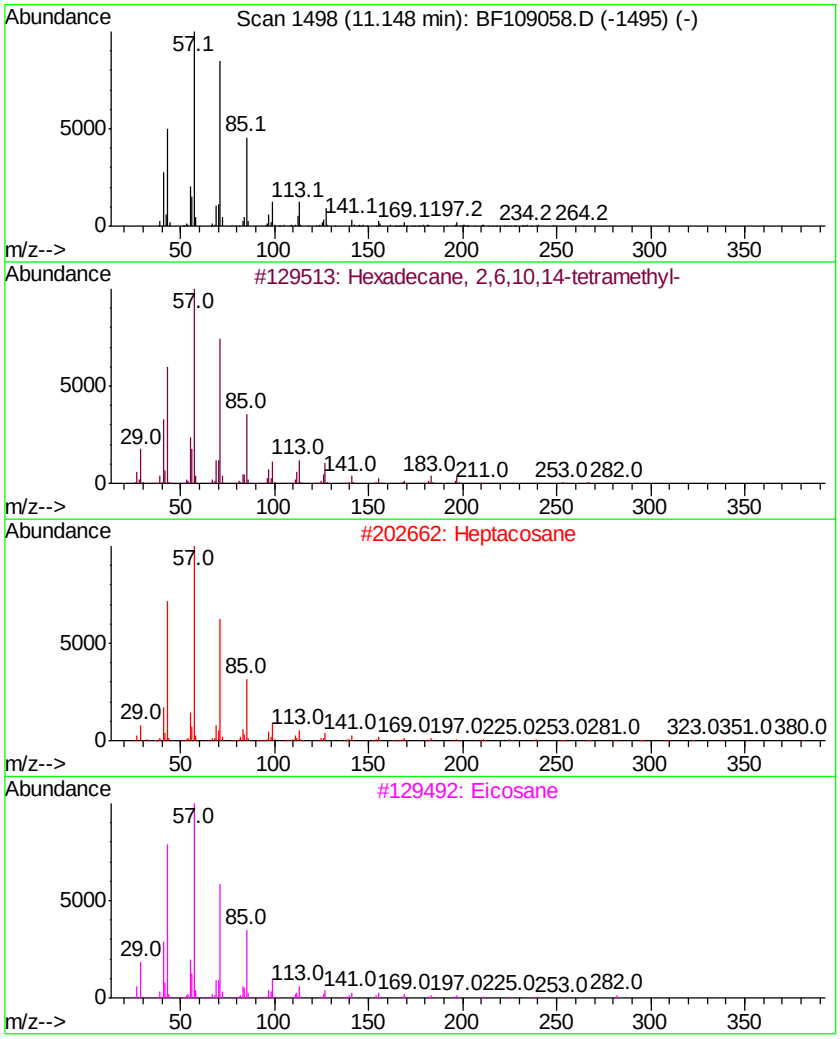
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

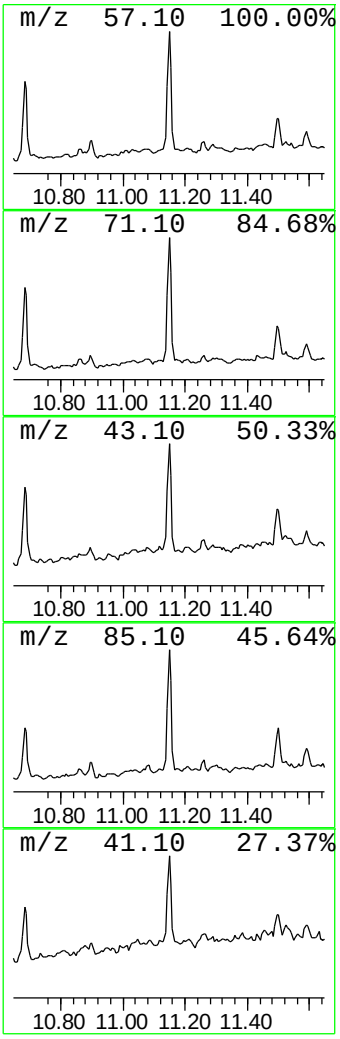
****

Peak Number 5 Hexadecane, 2,6,10,14-tetra... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.15	13.93 ng	524345	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	90
2	Heptacosane	380	C27H56	000593-49-7	86
3	Eicosane	282	C20H42	000112-95-8	86
4	Decane, 3-methyl-	156	C11H24	013151-34-3	83
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	80





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : RB12983RT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

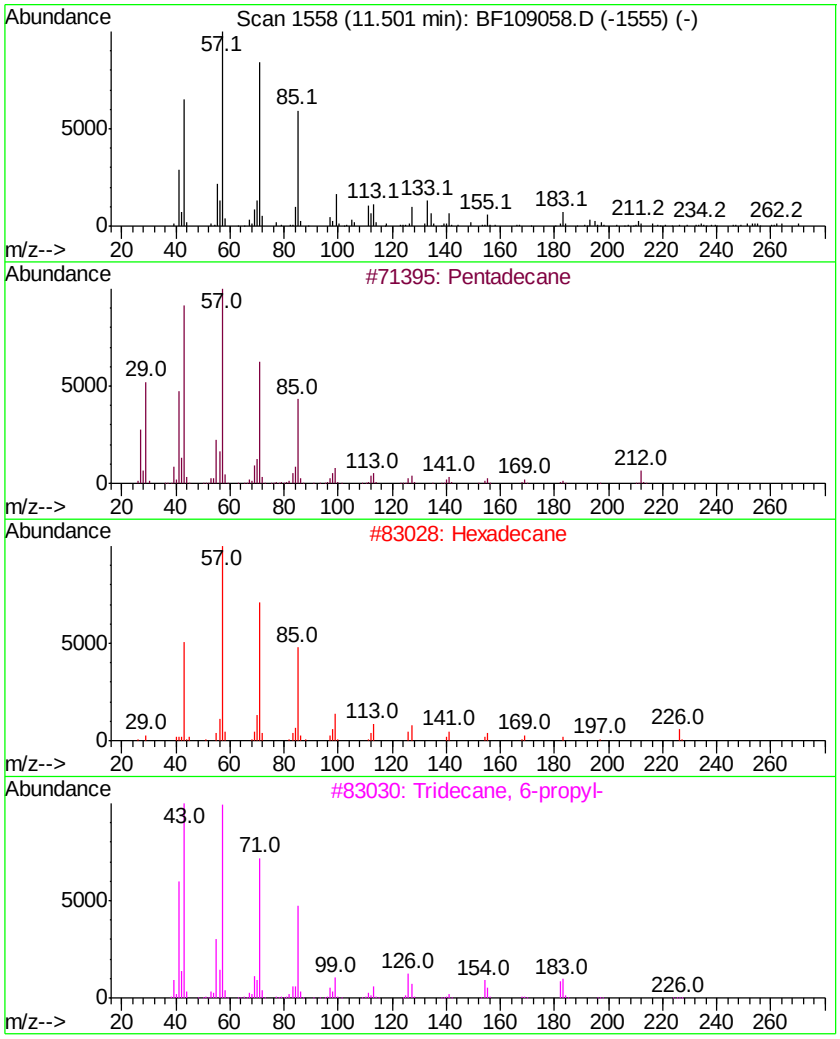
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

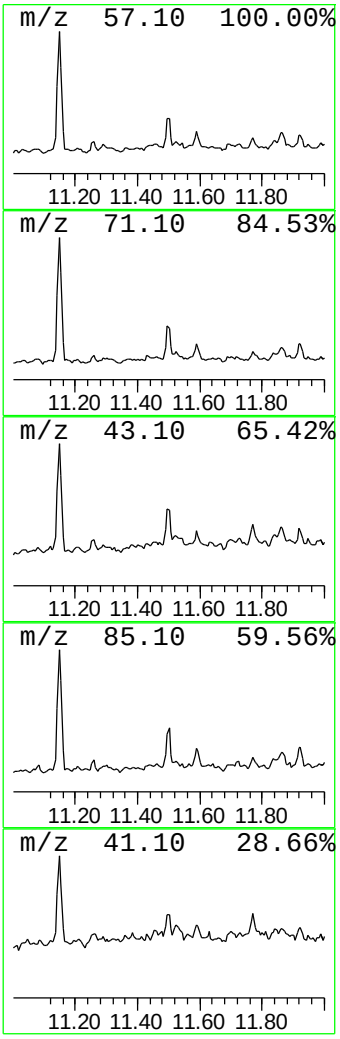
****

Peak Number 6 Pentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.50	3.85 ng	144859	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	91
2	Hexadecane	226	C16H34	000544-76-3	91
3	Tridecane, 6-propyl-	226	C16H34	055045-10-8	87
4	Hentriacontane	437	C31H64	000630-04-6	86
5	Triacontane	422	C30H62	000638-68-6	86





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Instrument : BNA_F
ClientSampleId : RB12983RT

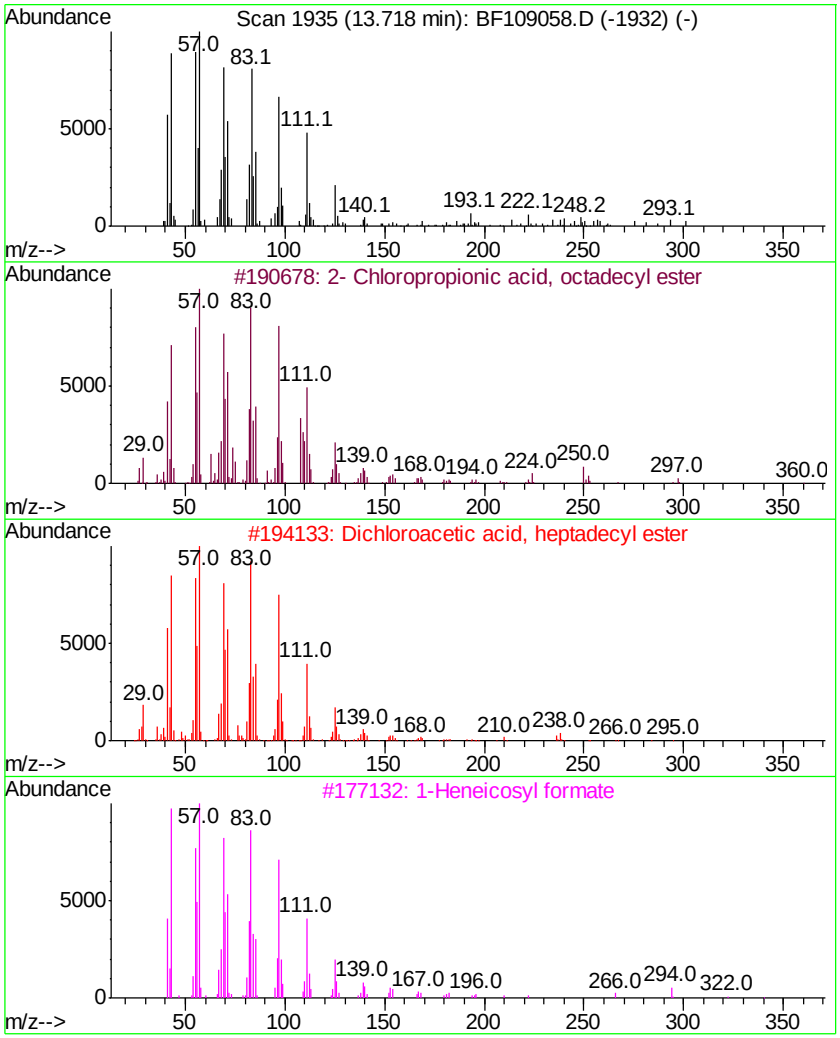
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

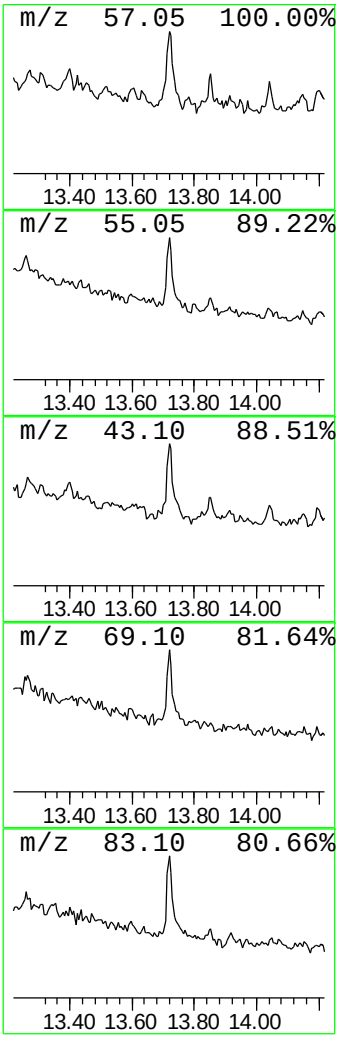
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2- Chloropropionic acid, oc... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	3.82 ng	219384	Chrysene-d12	13.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	90
4	1-Heneicosanol	312	C21H44O	015594-90-8	90
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	83





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

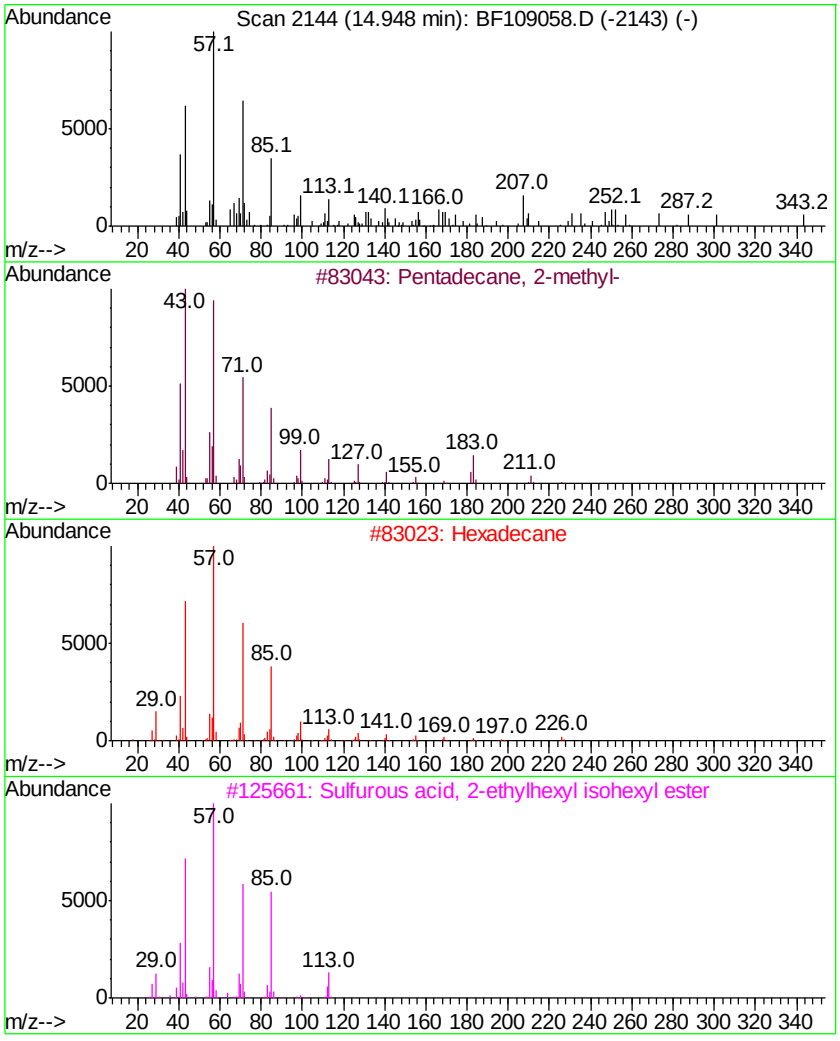
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

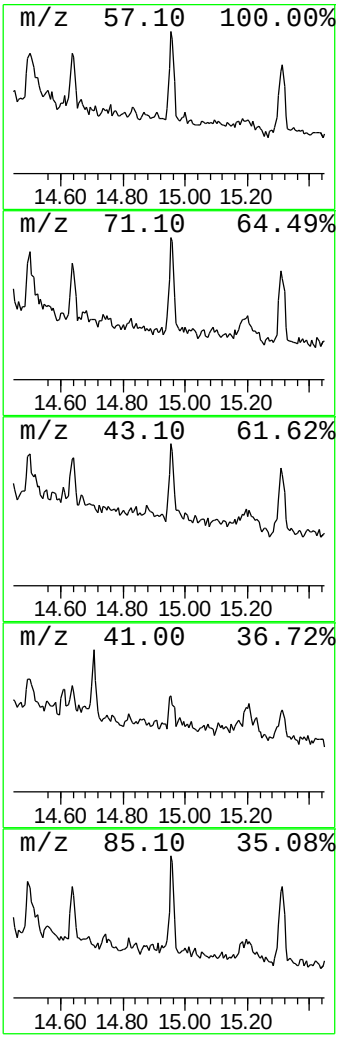
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	2.44 ng	87261	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2-methyl-	226	C16H34	001560-93-6	53
2	Hexadecane	226	C16H34	000544-76-3	53
3	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	49
4	Pentadecane	212	C15H32	000629-62-9	49
5	6,6-Diethylhexadecane	282	C20H42	1000360-41-4	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091718\
Data File : BF109058.D
Acq On : 17 Sep 2018 19:46
Operator : JU/SJ
Sample : J4946-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RB12983RT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.49	6.49	41.9	ng	1341430	1	6.72	640592	20.0
Undecane, 2,5-dim...	10.42	3.1	ng	130221	3	9.75	850753	20.0
Sulfurous acid, d...	10.68	9.3	ng	350483	4	11.23	753031	20.0
Hexadecane, 2,6,1...	11.15	13.9	ng	524345	4	11.23	753031	20.0
Pentadecane	11.50	3.9	ng	144859	4	11.23	753031	20.0
2- Chloropropioni...	13.72	3.8	ng	219384	5	13.85	1149700	20.0
Pentadecane, 2-me...	14.95	2.4	ng	87261	6	15.25	715340	20.0