LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090817\
Data File : BF098350.D
Acq On : 8 Sep 2017 15:06
Operator : SJ/JU
Sample : I5110-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2

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:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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	4.216	358	362	370	rBV	45197	61184	2.01%	0.211%
2	4.881	471	475	486	rBV	183728	286868	9.44%	0.990%
3	5.298	540	546	549	rBV	2542284	2792244	91.89%	9.636%
4	6.334	716	722	733	rBV	2538470	3038544	100.00%	10.486%
5	6.457	738	743	746	rBV	2605124	2778295	91.44%	9.588%
6	6.681	777	781	787	rVB	752545	616442	20.29%	2.127%
7	6.840	803	808	811	rBV	2253705	2167806	71.34%	7.481%
8	7.251	872	878	881	rBV	1836861	1846548	60.77%	6.372%
9	7.963	995	999	1002	rBV	977394	823354	27.10%	2.841%
10	9.045	1177	1183	1186	rBV	2987474	3024461	99.54%	10.437%
11	9.116	1191	1195	1198	rBV4	36486	45204	1.49%	0.156%
12	9.439	1245	1250	1253	rBV	333307	337368	11.10%	1.164%
13	9.475	1253	1256	1260	rVB4	32453	33222	1.09%	0.115%
14	9.581	1271	1274	1277	rBV3	76557	95945	3.16%	0.331%
15	9.622	1279	1281	1284	rVB	120141	104839	3.45%	0.362%
16	9.657	1284	1287	1290	rBV3	39003	49727	1.64%	0.172%
17	9.716	1290	1297	1300	rVV	1028091	966423	31.81%	3.335%
18	9.751	1300	1303	1306	rVB3	50936	61325	2.02%	0.212%
19	9.875	1322	1324	1326	rBV	35027	31961	1.05%	0.110%
20	9.975	1338	1341	1347	rBV	64610	72454	2.38%	0.250%
21	10.033	1348	1351	1352	rBV2	45019	41646	1.37%	0.144%
22	10.081	1357	1359	1362	rBV3	45083	43778	1.44%	0.151%
23	10.122	1362	1366	1368	rBV3	102449	107815	3.55%	0.372%
24	10.263	1386	1390	1395	rBV4	73450	140051	4.61%	0.483%
25	10.375	1406	1409	1414	rVB	81089	92097	3.03%	0.318%
26	10.422	1414	1417	1421	rVB4	38353	39800	1.31%	0.137%
27	10.510	1426	1432	1435	rBV	1679577	1762793	58.01%	6.083%
28	10.633	1449	1453	1456	rBV2	174281	249662	8.22%	0.862%
29	11.098	1530	1532	1536	rVB2	123246	141470	4.66%	0.488%
30	11.198	1546	1549	1551	rBV	945651	806480	26.54%	2.783%
31	11.222	1551	1553	1557	rVV	450953	351933	11.58%	1.214%
32	11.275	1559	1562	1565	rVB	84873	81524	2.68%	0.281%
33	11.727	1636	1639	1643	rVB	88760	95302	3.14%	0.329%
34	12.410	1751	1755	1758	rBV	512268	449161	14.78%	1.550%

LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090817\
Data File : BF098350.D
Acq On : 8 Sep 2017 15:06
Operator : SJ/JU
Sample : I5110-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2

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:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.633	1788	1793	1797	rBV	372252	388286	12.78%	1.340%
36	12.786	1814	1819	1822	rVB	2200026	2135933	70.29%	7.371%
37	13.474	1933	1936	1940	rVB	48454	54828	1.80%	0.189%
38	13.680	1968	1971	1979	rVB	236433	255773	8.42%	0.883%
39	13.833	1992	1997	1999	rBV2	625290	741119	24.39%	2.558%
40	13.857	1999	2001	2004	rVB	176370	133921	4.41%	0.462%
41	14.839	2164	2168	2171	rBV	179518	250579	8.25%	0.865%
42	14.915	2178	2181	2183	rBV	31891	33401	1.10%	0.115%
43	14.939	2183	2185	2188	rVB	43064	41167	1.35%	0.142%
44	15.121	2212	2216	2221	rVB	95870	116696	3.84%	0.403%
45	15.180	2222	2226	2231	rBV	132085	158694	5.22%	0.548%
46	15.239	2231	2236	2239	rBV	458148	561553	18.48%	1.938%
47	15.663	2304	2308	2311	rBV	36354	45544	1.50%	0.157%
48	15.715	2313	2317	2320	rVB5	26289	37667	1.24%	0.130%
49	16.121	2383	2386	2391	rVB2	26453	38950	1.28%	0.134%
50	16.586	2459	2465	2472	rVV2	68864	137924	4.54%	0.476%
51	16.662	2474	2478	2484	rVB4	30485	62849	2.07%	0.217%
52	16.992	2529	2534	2541	rVB	50879	98739	3.25%	0.341%
53	18.039	2706	2712	2718	rBV10	17328	46324	1.52%	0.160%

Sum of corrected areas: 28977673

LSC Report - Integrated Chromatogram

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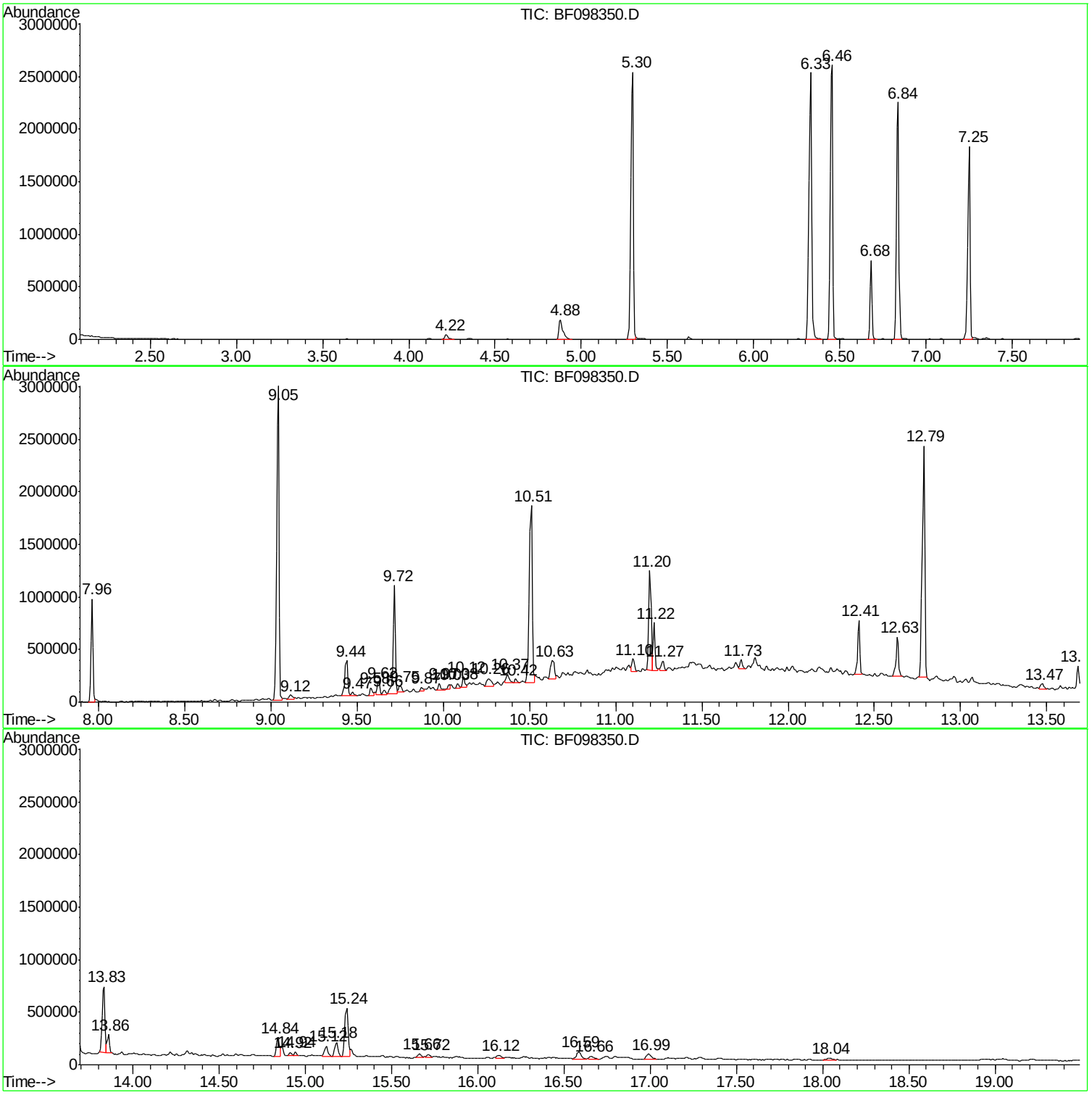
Sample : I5110-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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

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Data File : BF098350.D
Acq On : 8 Sep 2017 15:06
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Misc :
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Instrument : BNA_F
ClientSampleId : SP-2

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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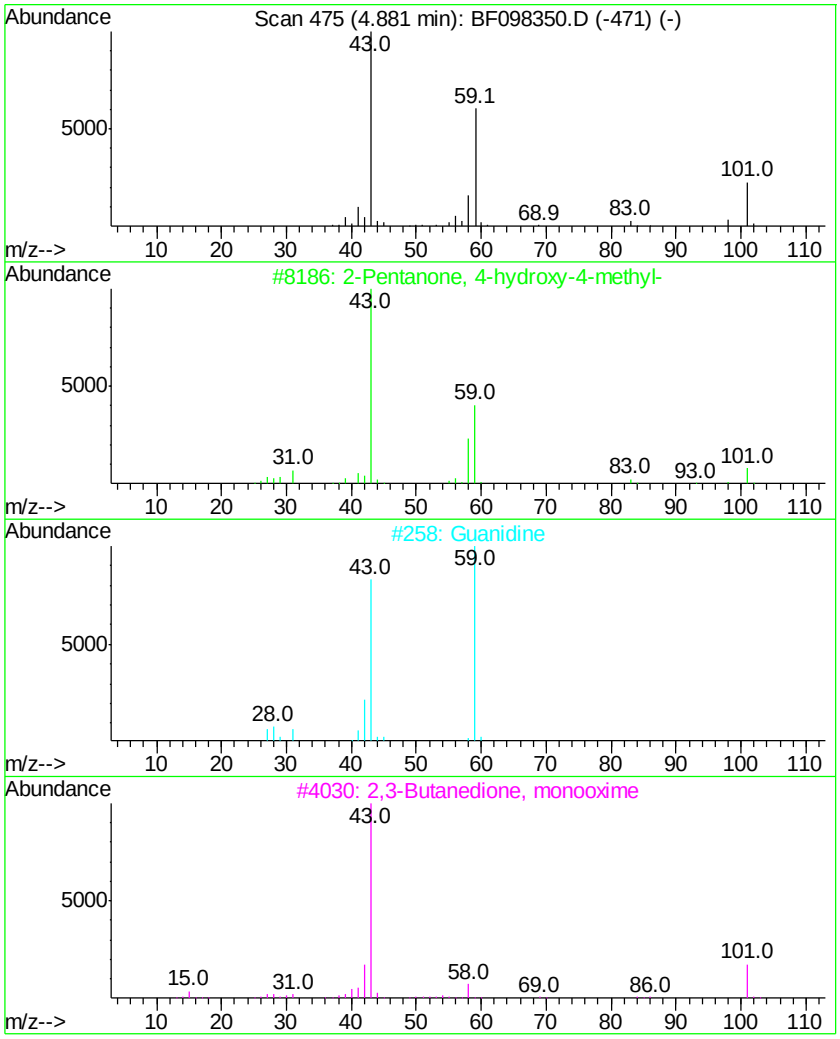
TIC Integration Parameters: LSCINT.P

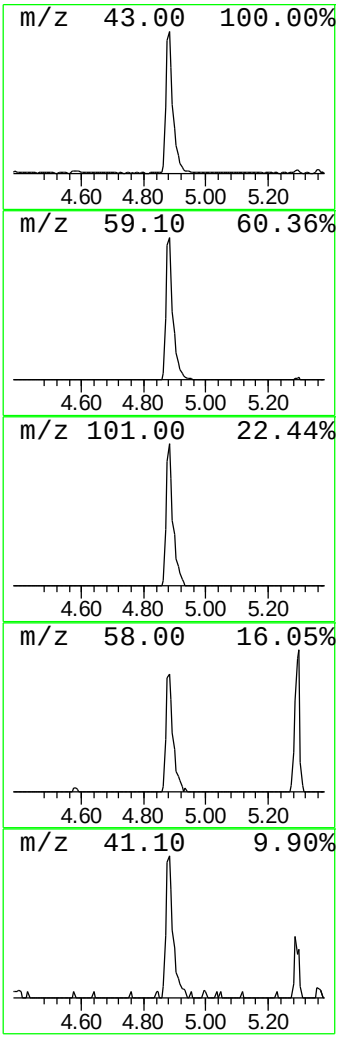
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	9.31 ng	286868	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Guanidine	59	CH5N3	000113-00-8	9
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Library Search Compound Report

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Acq On : 8 Sep 2017 15:06
Operator : SJ/JU
Sample : I5110-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

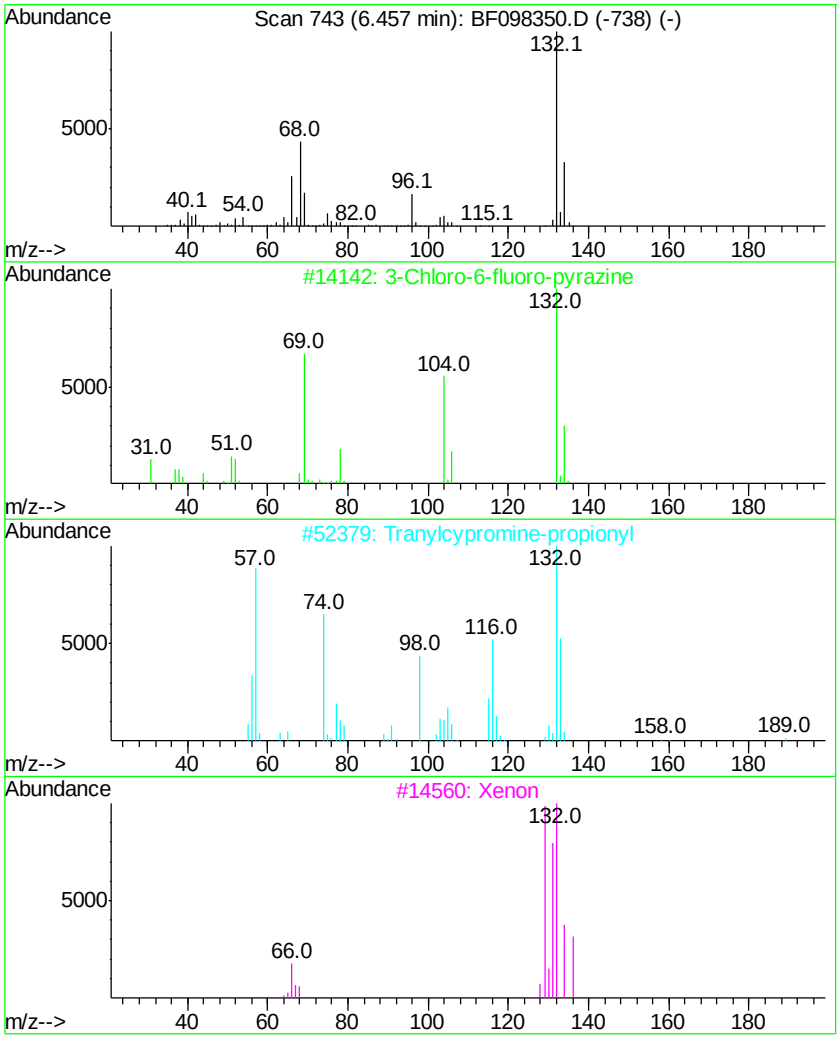
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

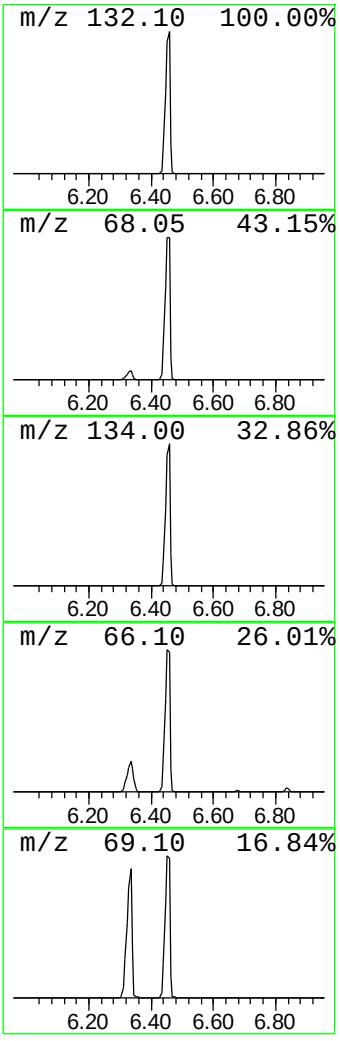
****

Peak Number 2 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	90.14 ng	2778300	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Xenon	132	Xe	007440-63-3	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Acq On : 8 Sep 2017 15:06
Operator : SJ/JU
Sample : I5110-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

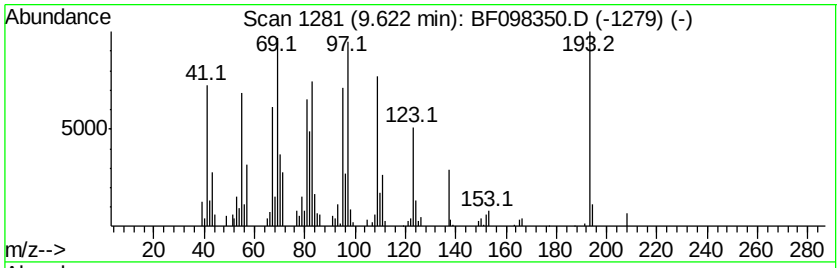
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

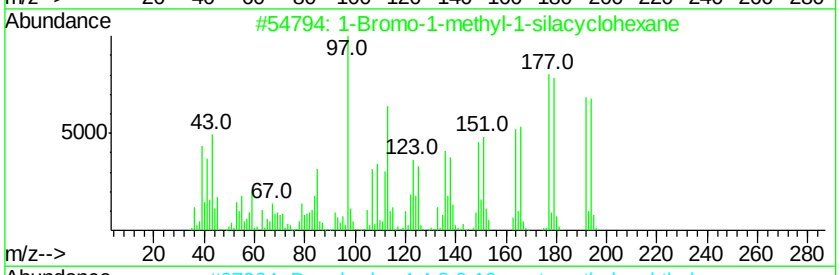
****

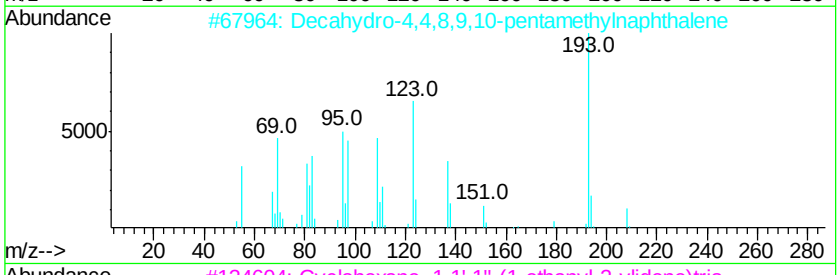
Peak Number 4 1-Bromo-1-methyl-1-silacycl... Concentration Rank 12

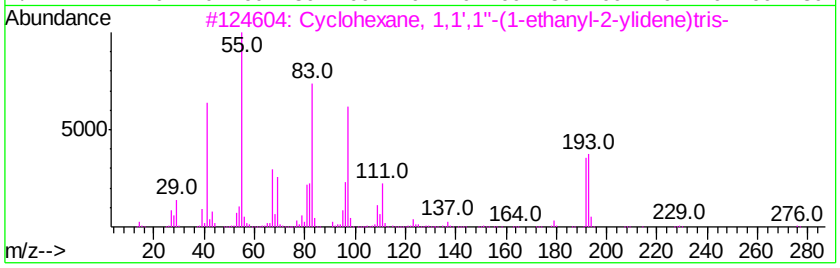
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.62	2.17 ng	104839	Acenaphthene-d10	9.72

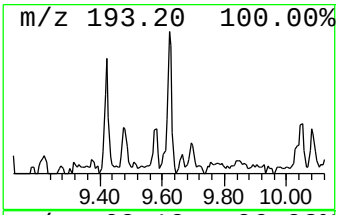
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Bromo-1-methyl-1-silacyclohexane	192	C6H13BrSi	085125-32-2	53
2	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	38
3	Cyclohexane, 1,1',1''-(1-ethanyl...	276	C20H36	055682-86-5	35
4	Cyclohexanecarboxylic acid, 4-pe...	292	C18H25FO2	079912-83-7	22
5	2-Pentene, 3-ethyl-4,4-dimethyl-	126	C9H18	053907-59-8	22

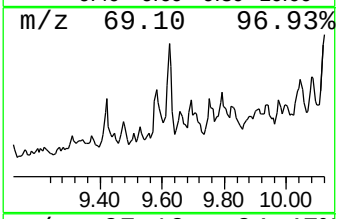


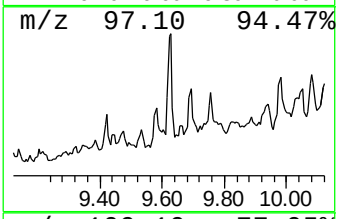


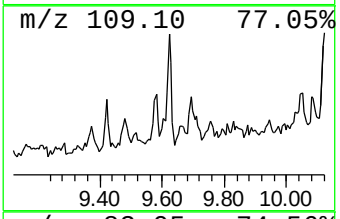


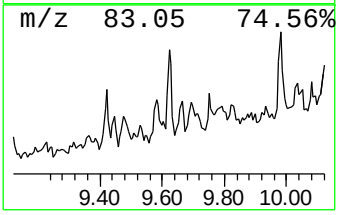












Library Search Compound Report

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Sample : I5110-04
Misc :
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Instrument : BNA_F
ClientSampleId : SP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

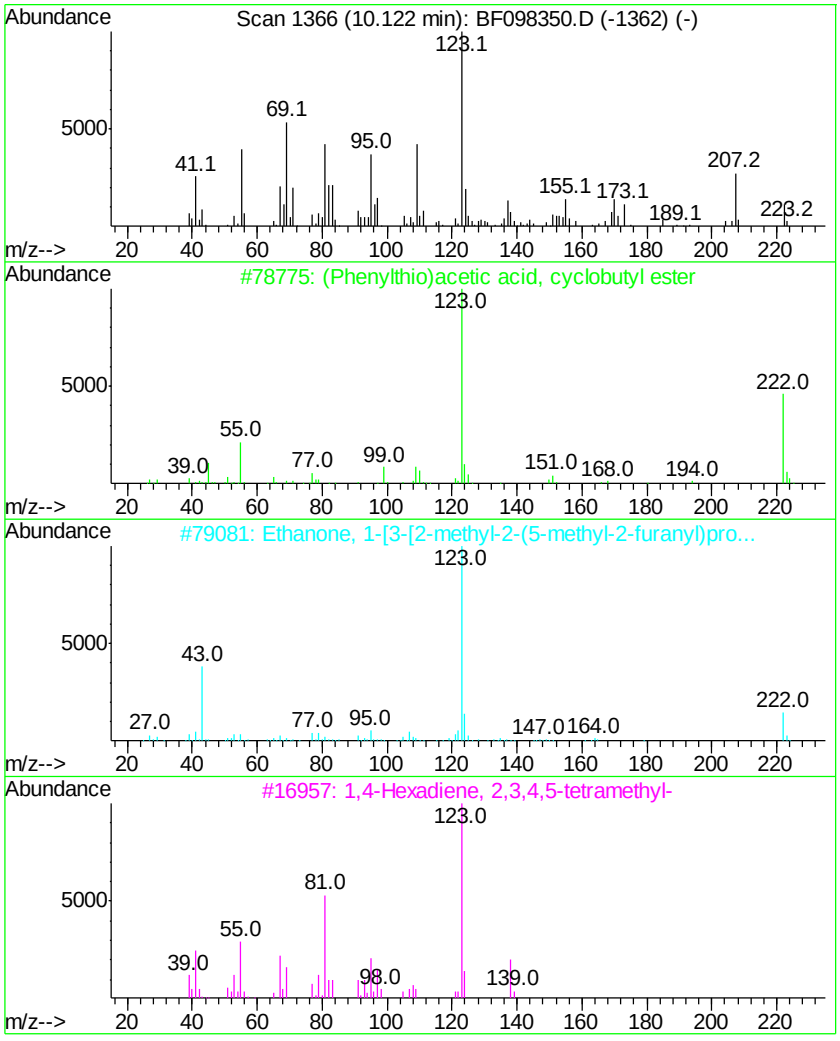
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

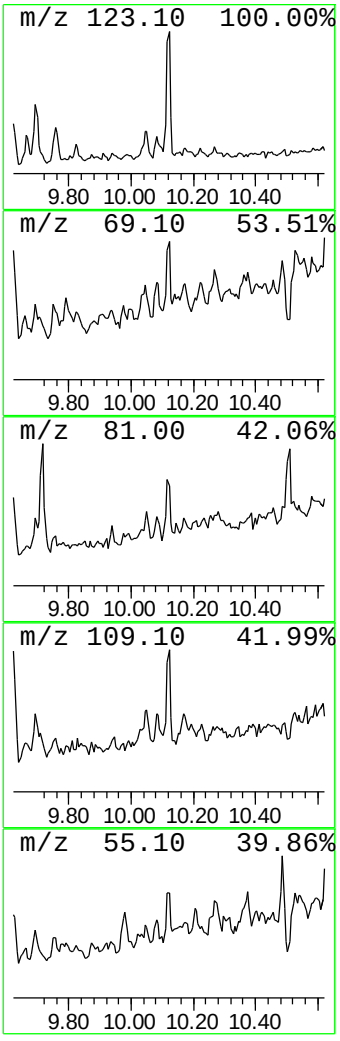
****

Peak Number 5 unknown10.12 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.12	2.23 ng	107815	Acenaphthene-d10	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Phenylthio)acetic acid, cyclobu...	222	C12H14O2S	1000299-95-5	41
2	Ethanone, 1-[3-[2-methyl-2-(5-me...	222	C13H18O3	080114-28-9	38
3	1,4-Hexadiene, 2,3,4,5-tetramethyl-	138	C10H18	051504-54-2	38
4	4-Fluorobenzoic acid, 2,2-dimeth...	210	C12H15FO2	069912-03-4	38
5	Bicyclo[4.1.0]heptane-7-carboxam...	222	C11H14N2OS	329912-72-3	38





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

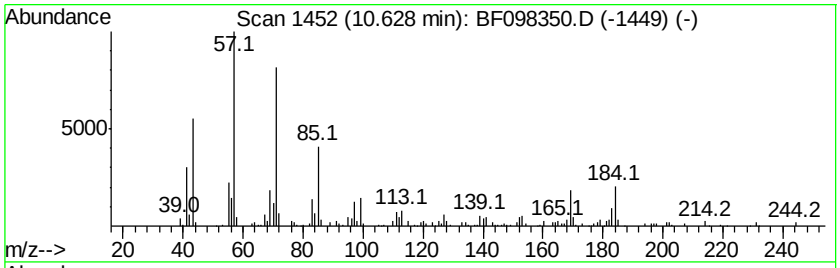
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

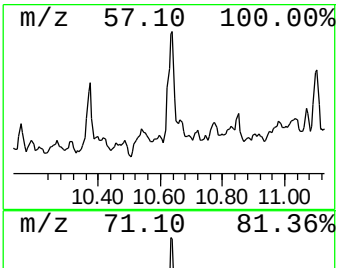
****

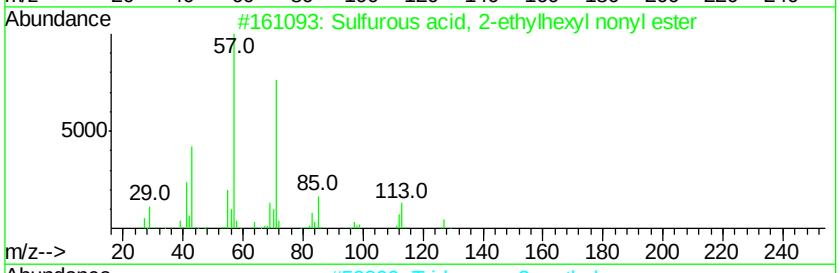
Peak Number 7 Sulfurous acid, 2-ethylhexy... Concentration Rank 5

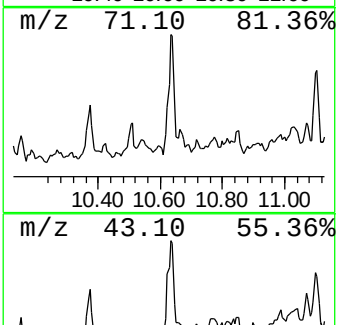
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	6.19 ng	249662	Phenanthrene-d10	11.20

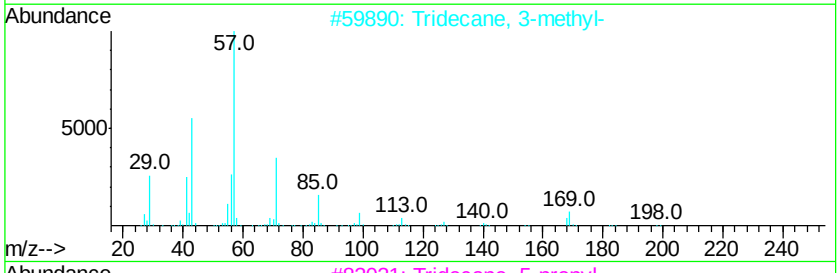
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1000309-19-2	72
2	Tridecane, 3-methyl-	198	C14H30	006418-41-3	59
3	Tridecane, 5-propyl-	226	C16H34	055045-11-9	59
4	Sulfurous acid, 2-ethylhexyl und...	348	C19H40O3S	1000309-19-4	59
5	Sulfurous acid, decyl 2-pentyl e...	292	C15H32O3S	1000309-15-9	53

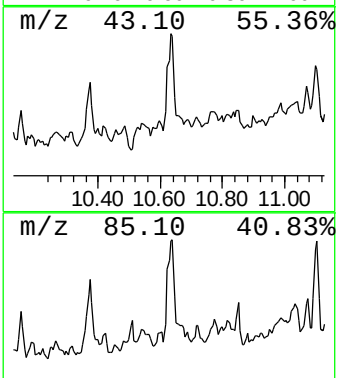


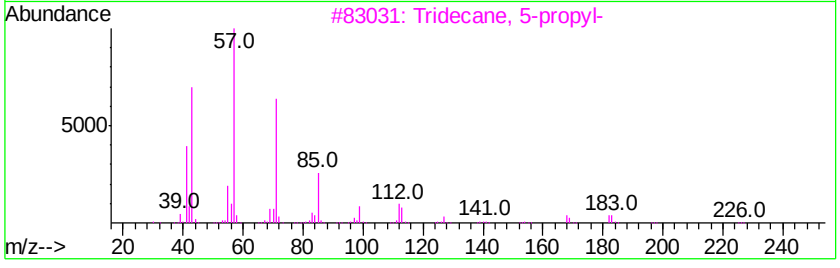


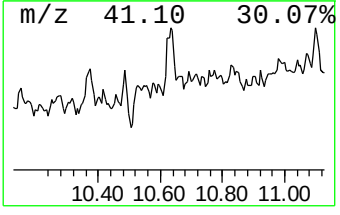












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ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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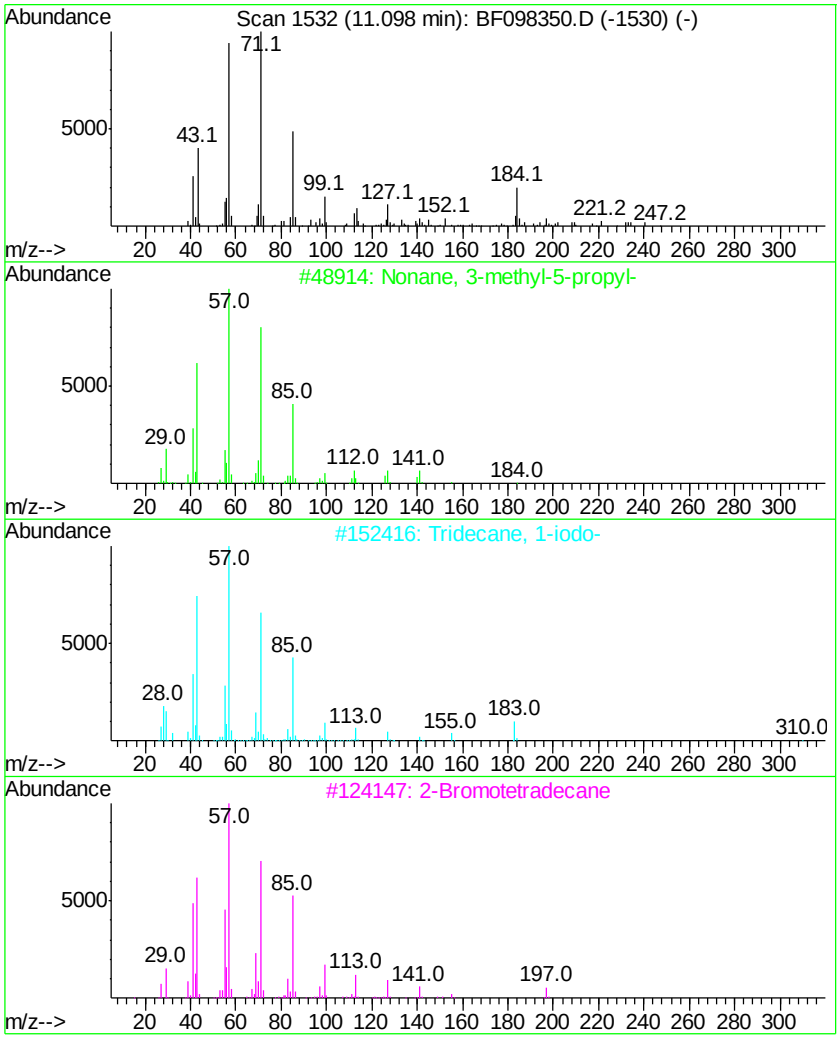
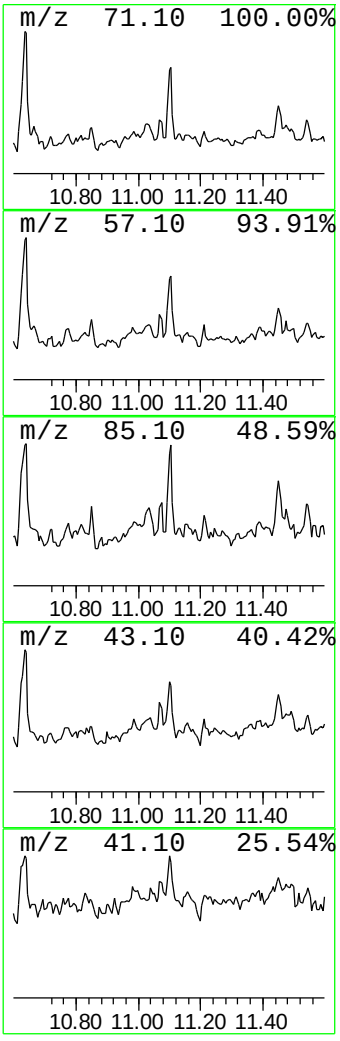
Peak Number 8 Nonane, 3-methyl-5-propyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.10	3.51 ng	141470	Phenanthrene-d10	11.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	64
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	59
3	2-Bromotetradecane	276	C14H29Br	074036-95-6	52
4	Heptadecane	240	C17H36	000629-78-7	49
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	49





Library Search Compound Report

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Acq On : 8 Sep 2017 15:06
Operator : SJ/JU
Sample : I5110-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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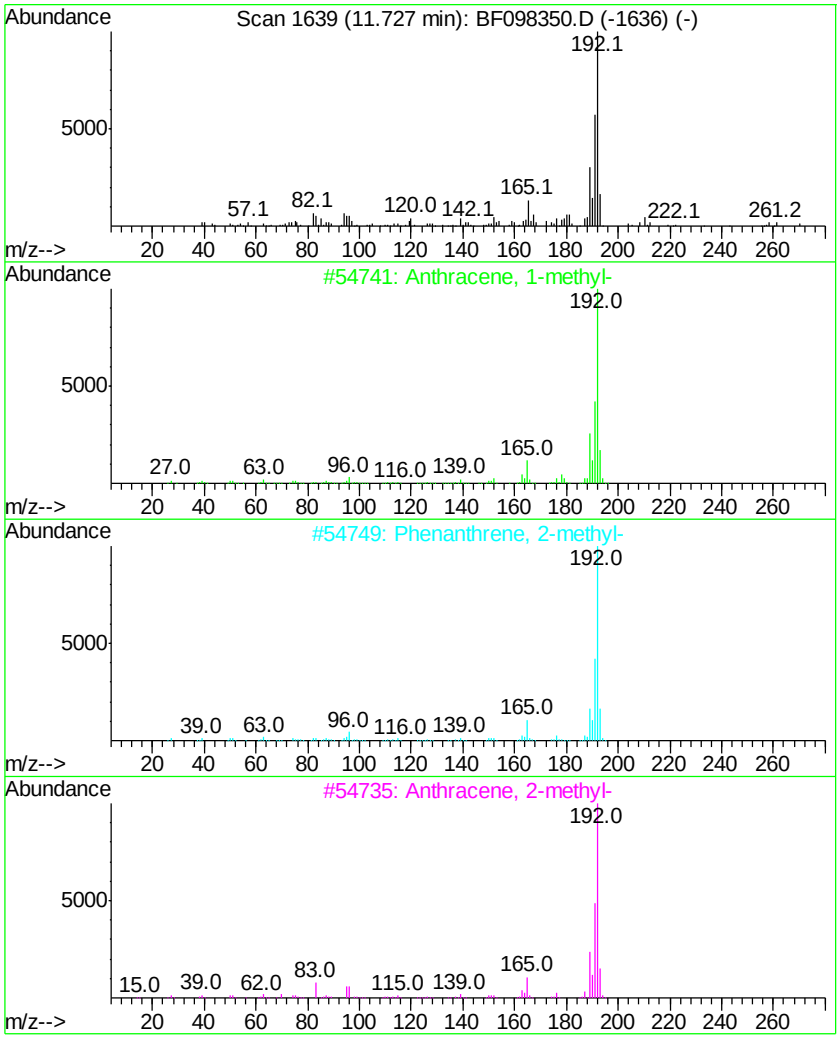
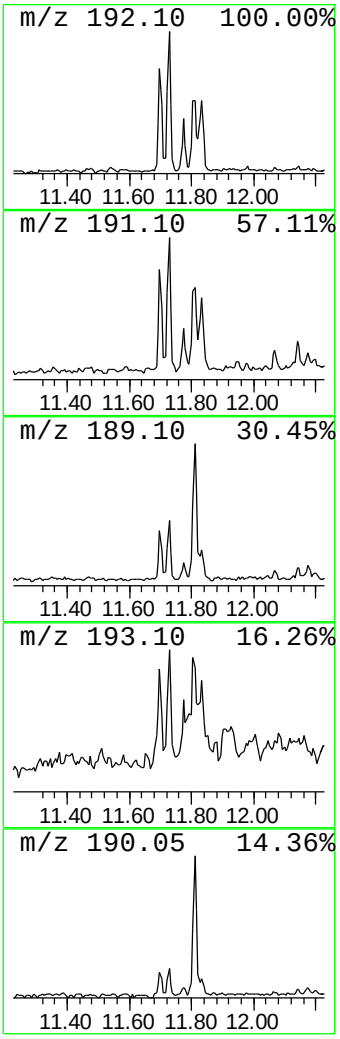
Peak Number 10 Anthracene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.73	2.36 ng	95302	Phenanthrene-d10	11.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	90
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	90
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	90
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	89





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Operator : SJ/JU
Sample : I5110-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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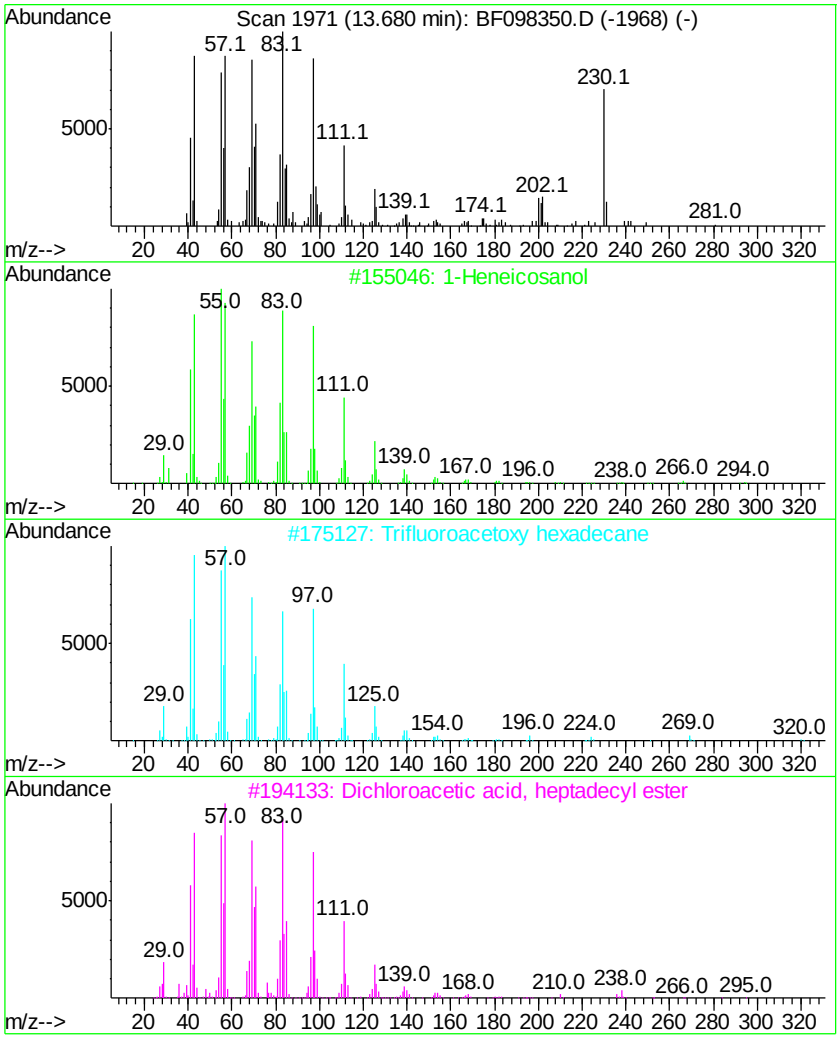
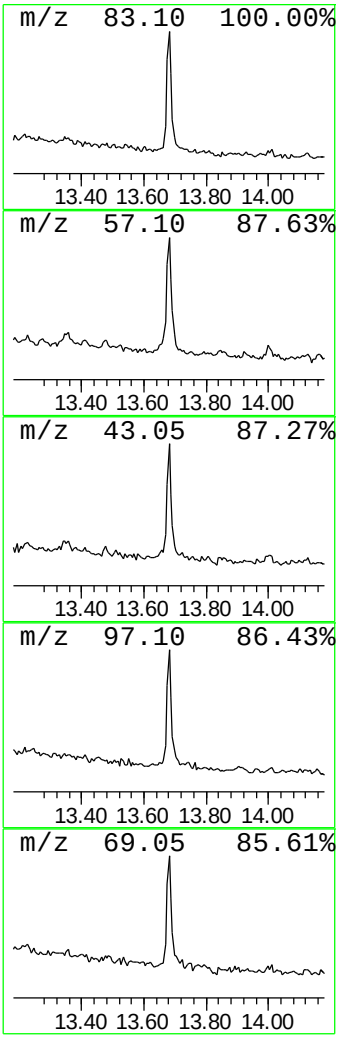
Peak Number 11 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	6.90 ng	255773	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	90





Library Search Compound Report

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Data File : BF098350.D
Acq On : 8 Sep 2017 15:06
Operator : SJ/JU
Sample : I5110-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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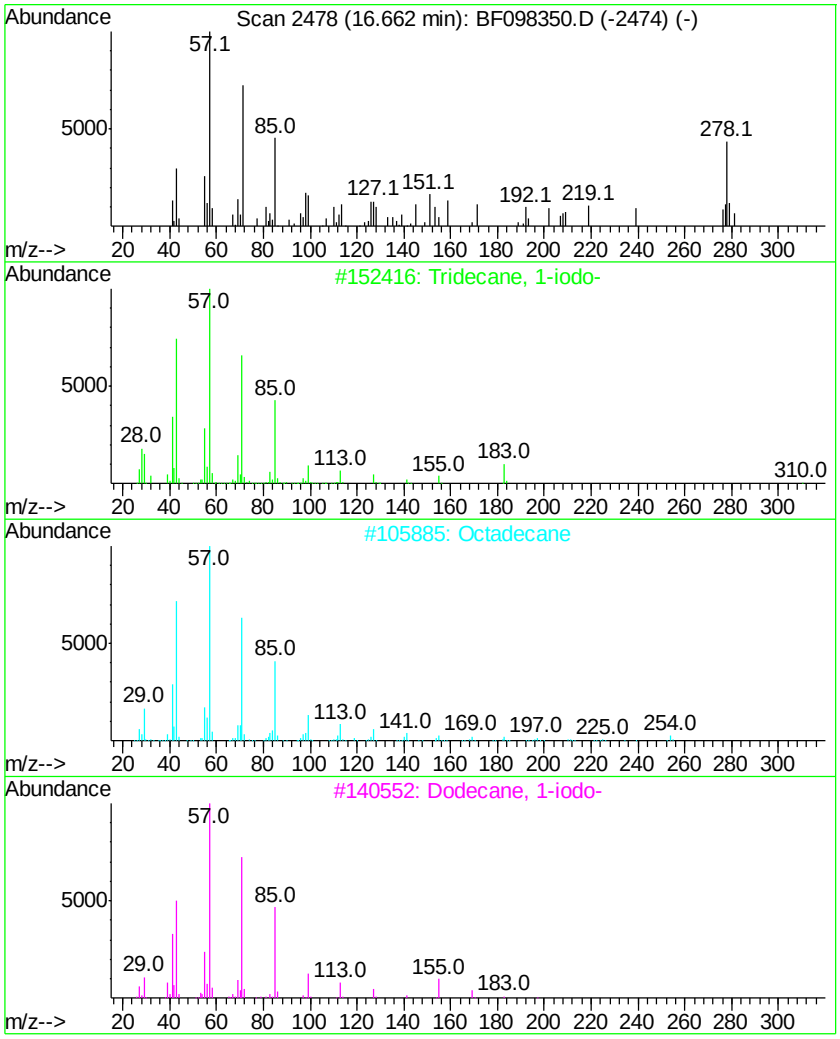
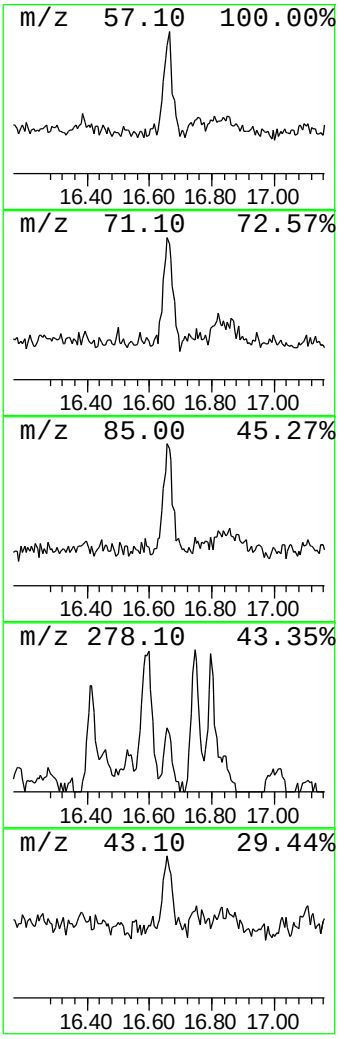
Peak Number 13 unknown16.66 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.66	2.24 ng	62849	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	38
2	Octadecane	254	C18H38	000593-45-3	35
3	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	35
4	3,7-Nonanedione, 5-(2-furanyl)-2...	278	C17H26O3	1000319-41-4	35
5	Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	35





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF090817\
Data File : BF098350.D
Acq On : 8 Sep 2017 15:06
Operator : SJ/JU
Sample : I5110-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2

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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
2-Pentanone, 4-hy...	4.88	9.3	ng	286868	1	6.68	616442	20.0
unknown6.46	6.46	90.1	ng	2778300	1	6.68	616442	20.0
1-Bromo-1-methyl-...	9.62	2.2	ng	104839	3	9.72	966423	20.0
unknown10.12	10.12	2.2	ng	107815	3	9.72	966423	20.0
Sulfurous acid, 2...	10.63	6.2	ng	249662	4	11.20	806480	20.0
Nonane, 3-methyl-...	11.10	3.5	ng	141470	4	11.20	806480	20.0
Anthracene, 1-met...	11.73	2.4	ng	95302	4	11.20	806480	20.0
1-Heneicosanol	13.68	6.9	ng	255773	5	13.83	741119	20.0
unknown16.66	16.66	2.2	ng	62849	6	15.24	561553	20.0