LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091217\
Data File : BF098467.D
Acq On : 12 Sep 2017 23:06
Operator : SJ/JU
Sample : I5140-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-10-10.5-21

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-BF091117.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	3.587	248	255	265	rBV	360653	577254	10.45%	1.254%
2	4.851	467	470	482	rBV	335438	548161	9.92%	1.190%
3	5.275	538	542	557	rBV	5104733	5463117	98.90%	11.864%
4	6.316	714	719	730	rBV	4684146	5523821	100.00%	11.996%
5	6.440	735	740	743	rBV	5218977	5146334	93.17%	11.176%
6	6.663	774	778	784	rBV	1599660	1342256	24.30%	2.915%
7	6.816	800	804	808	rBV	3818631	3793241	68.67%	8.237%
8	7.092	849	851	866	rVB	126959	173138	3.13%	0.376%
9	7.234	870	875	878	rBV	3437604	3137141	56.79%	6.813%
10	7.710	950	956	960	rBV2	51065	69519	1.26%	0.151%
11	7.945	990	996	998	rBV	2089922	1698332	30.75%	3.688%
12	7.969	998	1000	1005	rVB	219412	202701	3.67%	0.440%
13	8.657	1113	1117	1120	rVB	80179	63229	1.14%	0.137%
14	9.022	1174	1179	1182	rBV	5139183	4526912	81.95%	9.831%
15	9.416	1243	1246	1250	rVB	649944	513019	9.29%	1.114%
16	9.633	1279	1283	1286	rVB	61413	60151	1.09%	0.131%
17	9.692	1286	1293	1297	rBV	1630676	1532109	27.74%	3.327%
18	10.128	1364	1367	1370	rVB	71568	60356	1.09%	0.131%
19	10.351	1399	1405	1411	rBV	43942	66765	1.21%	0.145%
20	10.486	1422	1428	1439	rBV	2213351	2129353	38.55%	4.624%
21	10.604	1445	1448	1454	rBV	111883	150923	2.73%	0.328%
22	11.045	1520	1523	1526	rBV3	80865	80488	1.46%	0.175%
23	11.175	1540	1545	1548	rBV	1552446	1313412	23.78%	2.852%
24	11.198	1548	1549	1552	rVV	134997	86131	1.56%	0.187%
25	11.251	1555	1558	1561	rVB	53669	59405	1.08%	0.129%
26	12.145	1708	1710	1715	rBV3	47859	73700	1.33%	0.160%
27	12.386	1748	1751	1754	rBV	179682	141126	2.55%	0.306%
28	12.610	1787	1789	1792	rVB	164307	139394	2.52%	0.303%
29	12.663	1796	1798	1804	rVB2	86042	78933	1.43%	0.171%
30	12.757	1810	1814	1818	rBV	2984320	2946715	53.35%	6.399%
31	13.480	1935	1937	1943	rVB2	102461	97298	1.76%	0.211%
32	13.533	1943	1946	1949	rBV3	125719	140351	2.54%	0.305%
33	13.657	1964	1967	1973	rVB	193714	209330	3.79%	0.455%
34	13.710	1973	1976	1979	rBV	317760	277451	5.02%	0.603%

LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091217\
Data File : BF098467.D
Acq On : 12 Sep 2017 23:06
Operator : SJ/JU
Sample : I5140-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-10-10.5-21

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-BF091117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.810	1987	1993	1996	rBV2	1281380	1477607	26.75%	3.209%
36	13.833	1996	1997	2003	rVB	115579	92434	1.67%	0.201%
37	13.974	2019	2021	2024	rVB2	82210	80647	1.46%	0.175%
38	14.080	2036	2039	2045	rVB4	86673	151744	2.75%	0.330%
39	14.280	2071	2073	2077	rBV2	102157	114275	2.07%	0.248%
40	14.639	2132	2134	2137	rVB	174184	146803	2.66%	0.319%
41	15.151	2219	2221	2226	rVB	108974	117101	2.12%	0.254%
42	15.210	2227	2231	2240	rVB	738271	964419	17.46%	2.094%
43	15.445	2268	2271	2276	rVB	158228	201067	3.64%	0.437%
44	15.504	2278	2281	2290	rVB	173560	281296	5.09%	0.611%

Sum of corrected areas: 46048959

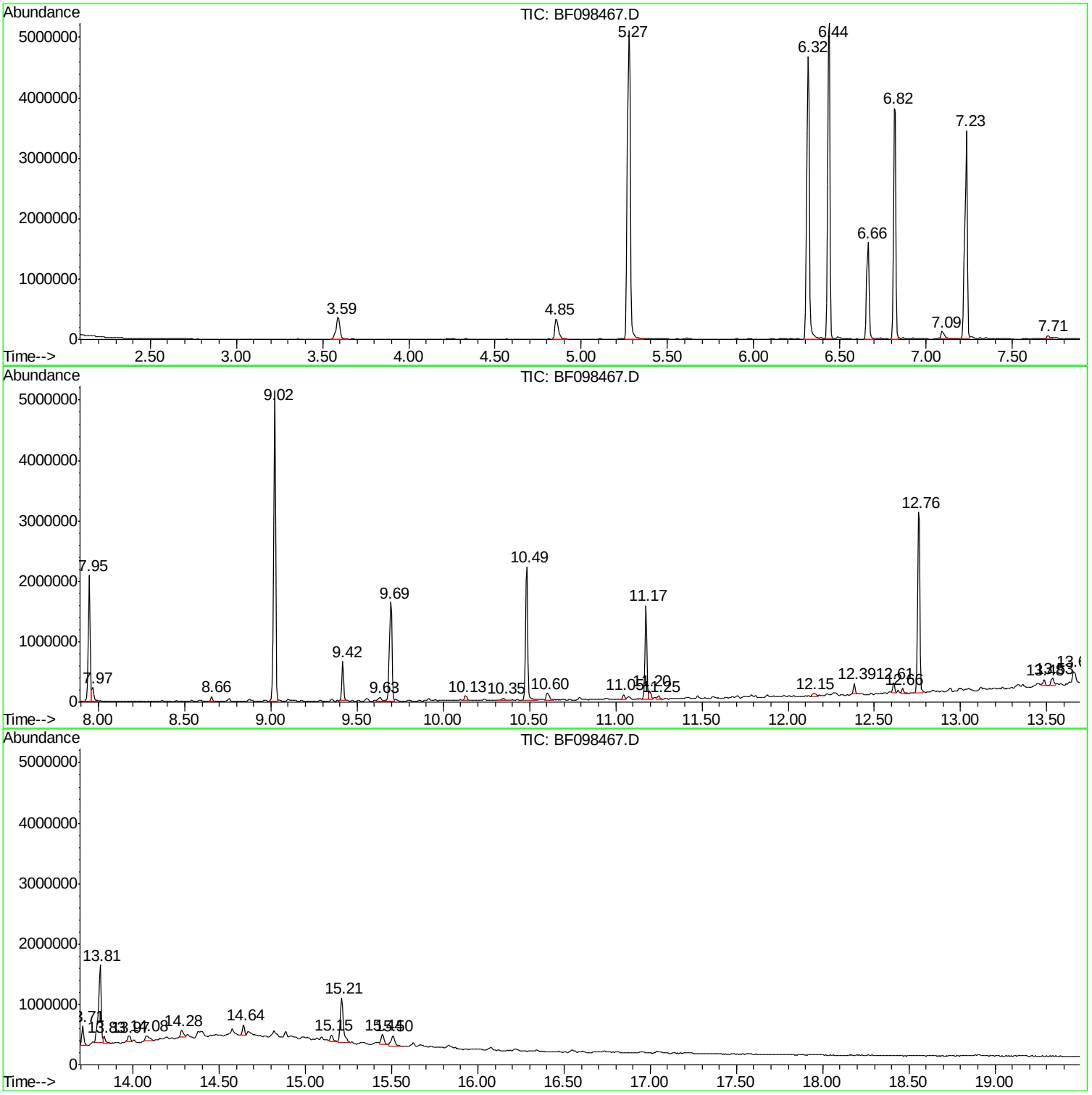
LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091217\
Data File : BF098467.D
Acq On : 12 Sep 2017 23:06
Operator : SJ/JU
Sample : I5140-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RL-10-10.5-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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Data File : BF098467.D
Acq On : 12 Sep 2017 23:06
Operator : SJ/JU
Sample : I5140-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-10-10.5-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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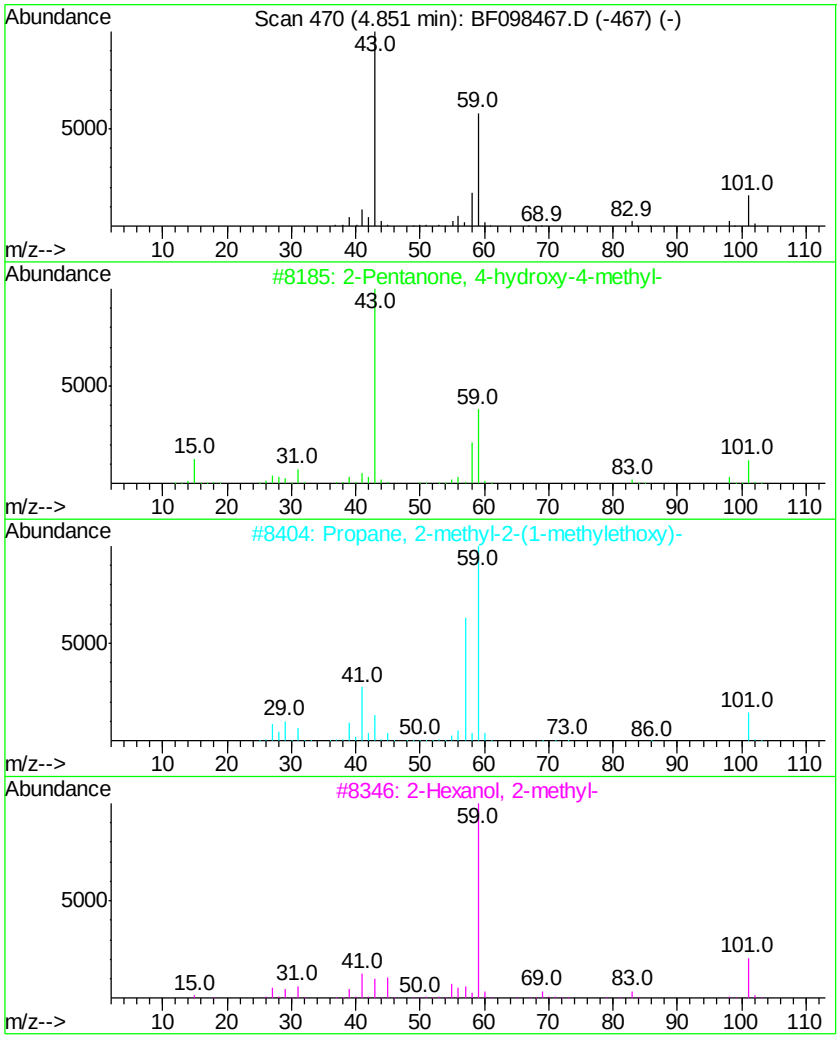
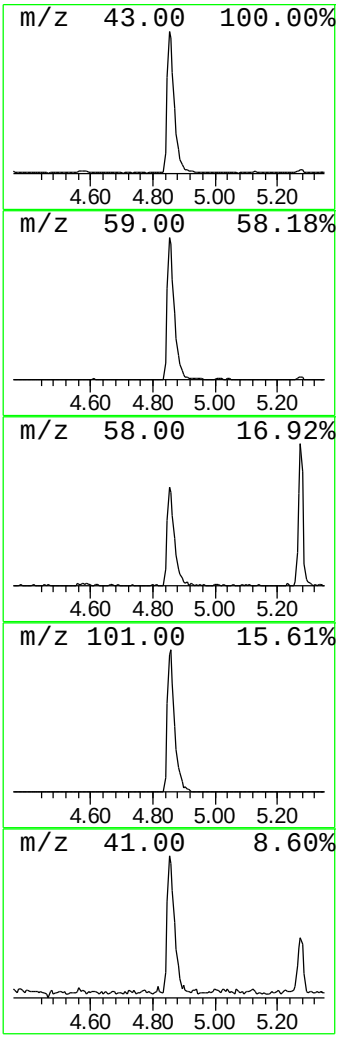
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	8.17 ng	548161	1,4-Dichlorobenzene-d4	6.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091217\
Data File : BF098467.D
Acq On : 12 Sep 2017 23:06
Operator : SJ/JU
Sample : I5140-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-10-10.5-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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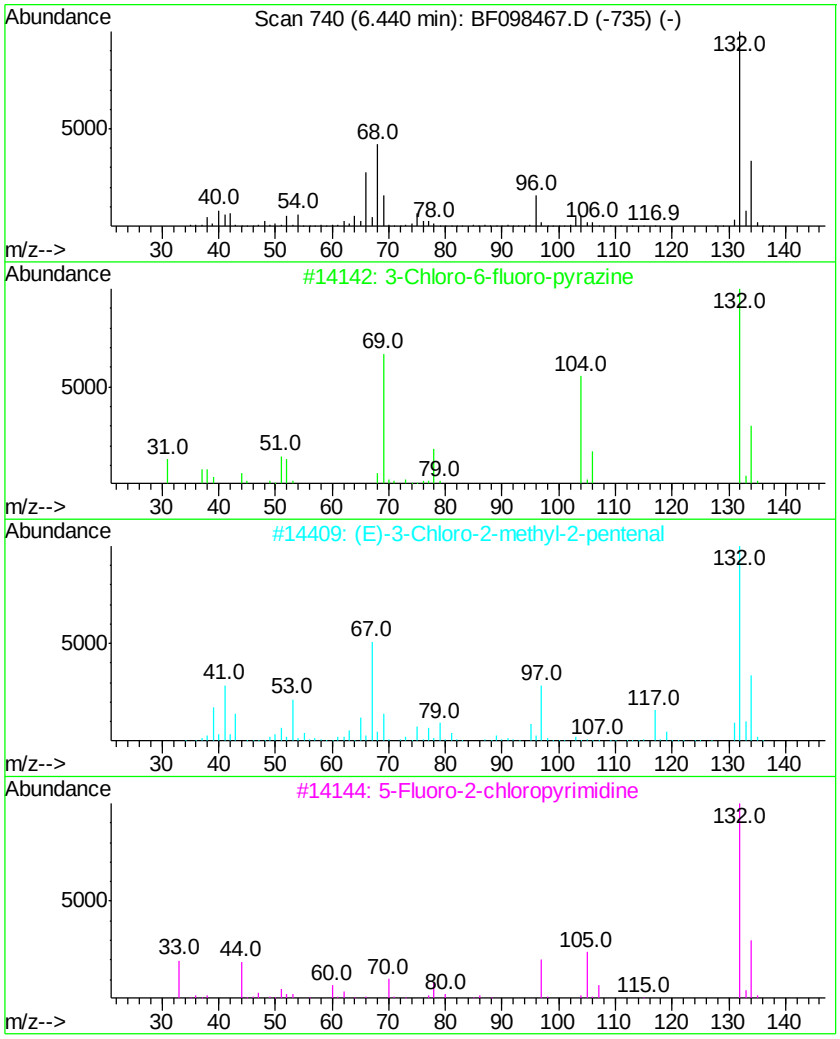
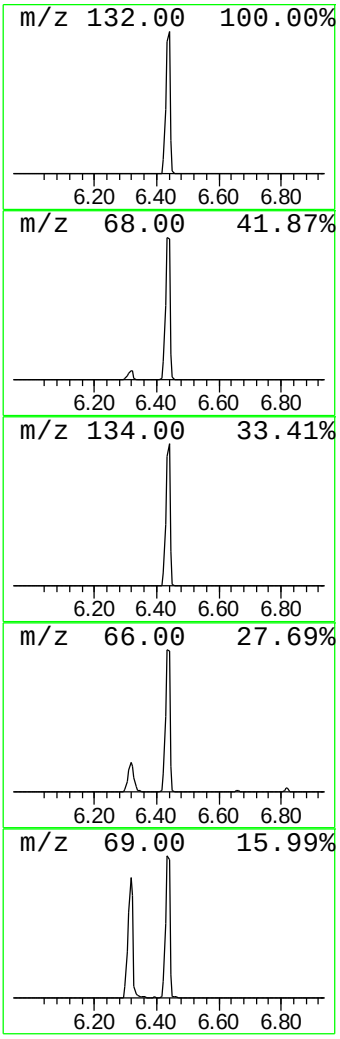
Peak Number 3 unknown6.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	76.68 ng	5146330	1,4-Dichlorobenzene-d4	6.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





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Data File : BF098467.D
Acq On : 12 Sep 2017 23:06
Operator : SJ/JU
Sample : I5140-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-10-10.5-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

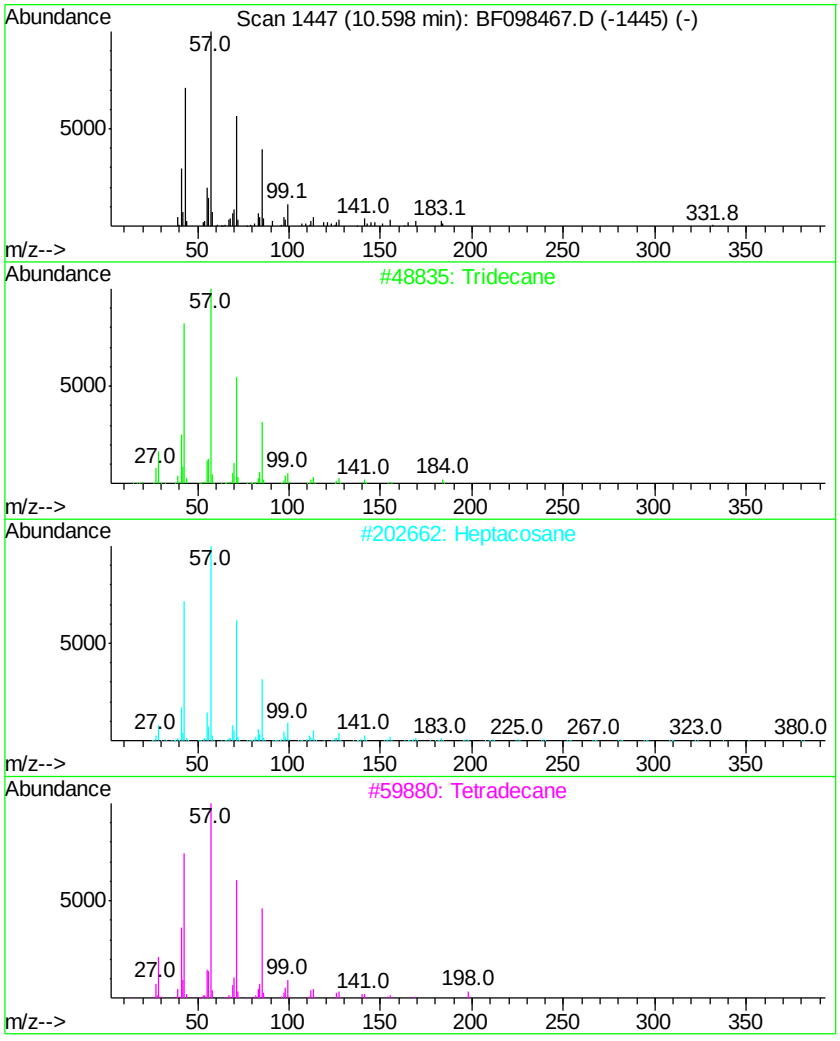
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

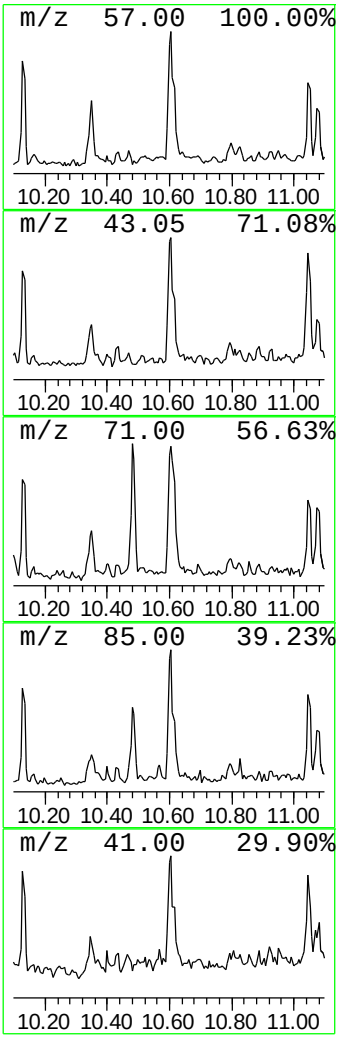
****

Peak Number 5 Tridecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	2.30 ng	150923	Phenanthrene-d10	11.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	87
2	Heptacosane	380	C27H56	000593-49-7	83
3	Tetradecane	198	C14H30	000629-59-4	80
4	Eicosane	282	C20H42	000112-95-8	68
5	Tridecane, 7-hexyl-	268	C19H40	007225-66-3	64





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Data File : BF098467.D
Acq On : 12 Sep 2017 23:06
Operator : SJ/JU
Sample : I5140-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-10-10.5-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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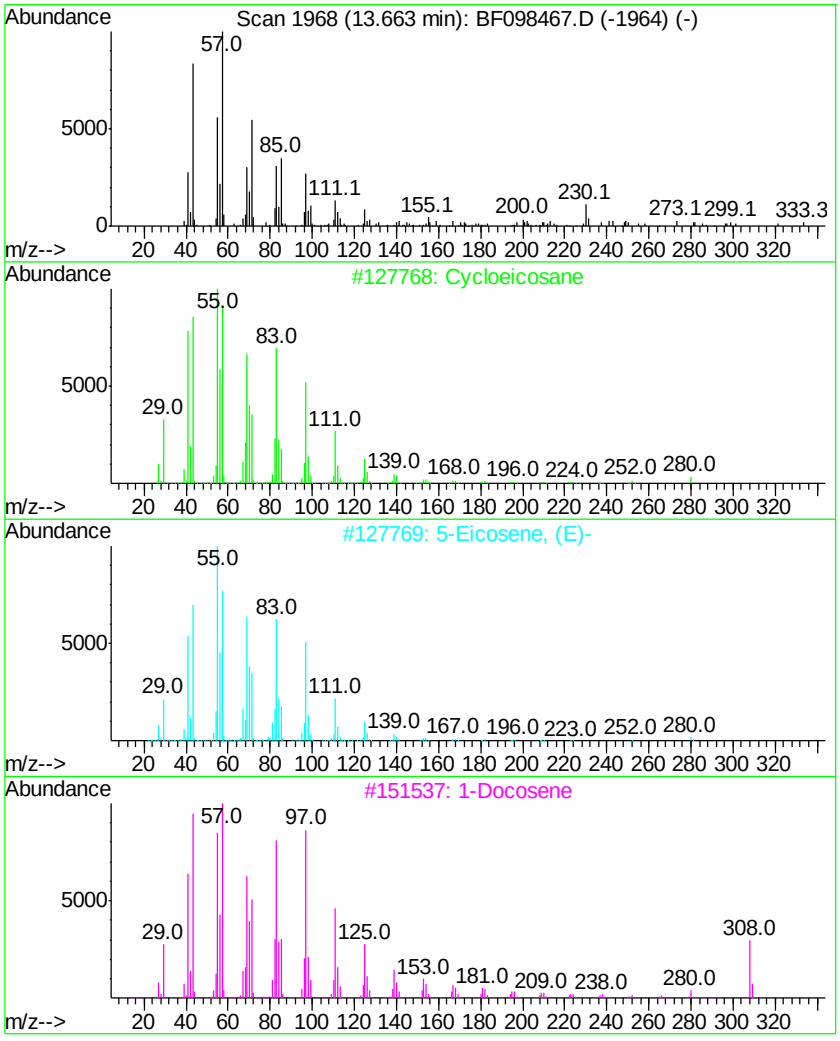
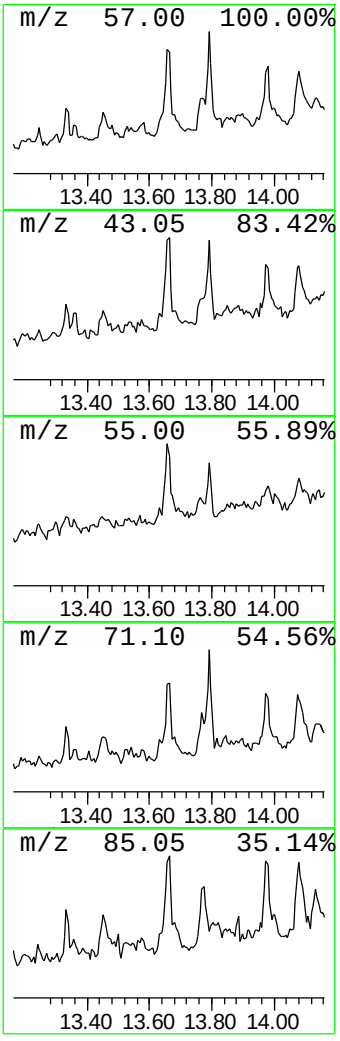
Peak Number 6 Cycloeicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	2.83 ng	209330	Chrysene-d12	13.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloeicosane	280	C20H40	000296-56-0	97
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	96
3	1-Docosene	308	C22H44	001599-67-3	95
4	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	95
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	93





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Acq On : 12 Sep 2017 23:06
Operator : SJ/JU
Sample : I5140-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-10-10.5-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

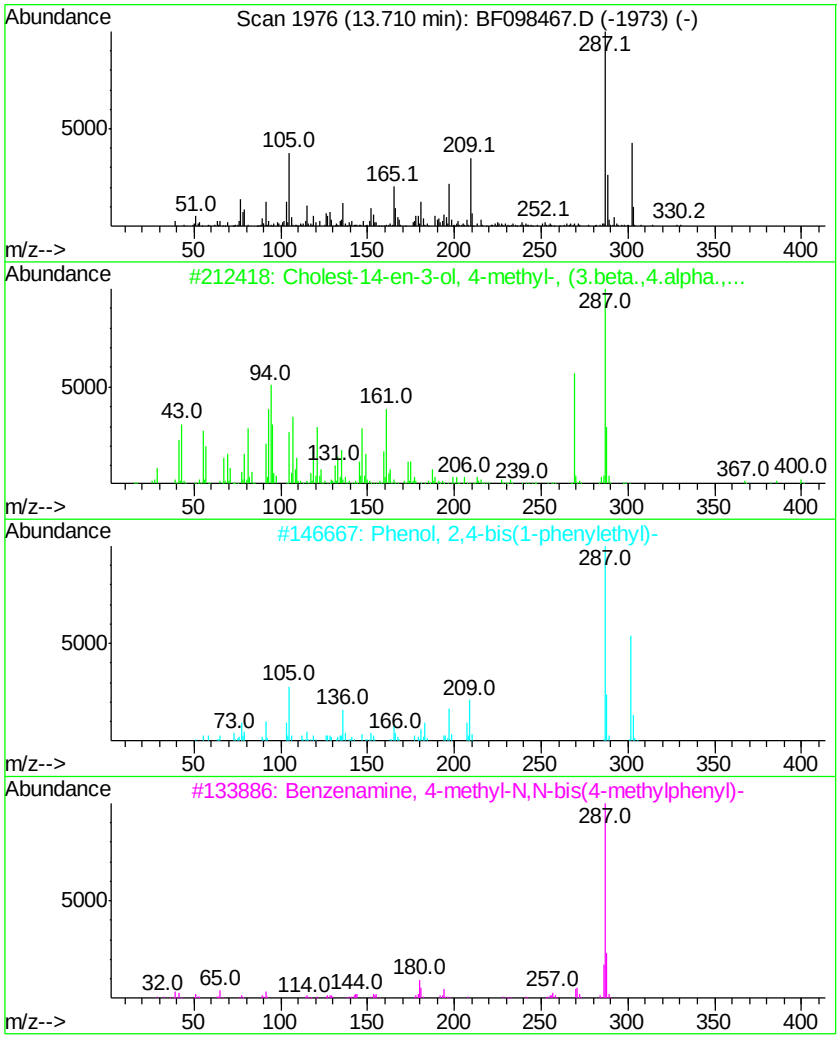
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

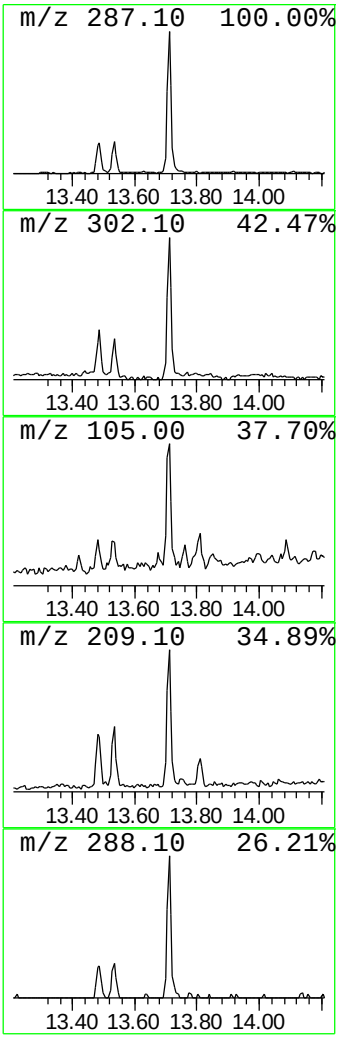
****

Peak Number 7 Cholest-14-en-3-ol, 4-methy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	3.76 ng	277451	Chrysene-d12	13.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholest-14-en-3-ol, 4-methyl-, (...	400	C28H48O	064130-22-9	95
2	Phenol, 2,4-bis(1-phenylethyl)-	302	C22H22O	002769-94-0	87
3	Benzenamine, 4-methyl-N,N-bis(4-...	287	C21H21N	1000327-28-1	38
4	6-Trifluoromethyl-benzo[4,5]imid...	287	C15H8F3N3	1000317-89-2	38
5	2-(3-Bromo-phenyl)-2,3-dihydro-i...	287	C14H10BrNO	004778-88-5	35





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Data File : BF098467.D
Acq On : 12 Sep 2017 23:06
Operator : SJ/JU
Sample : I5140-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-10-10.5-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

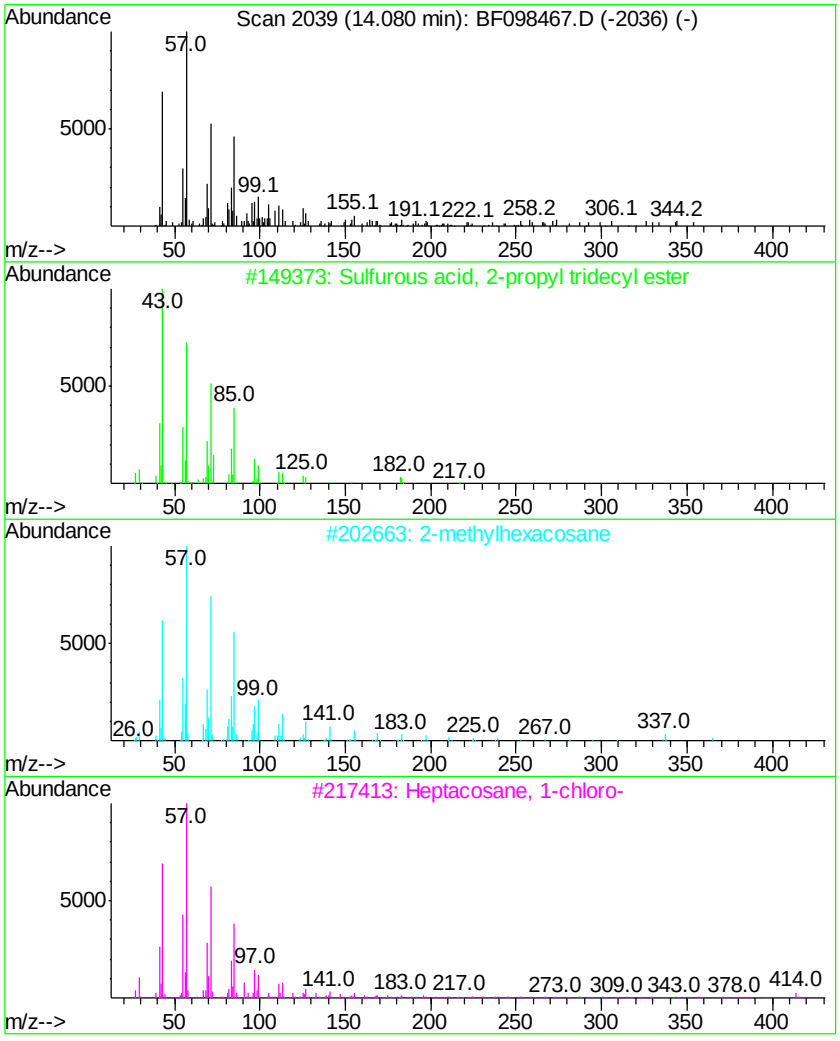
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

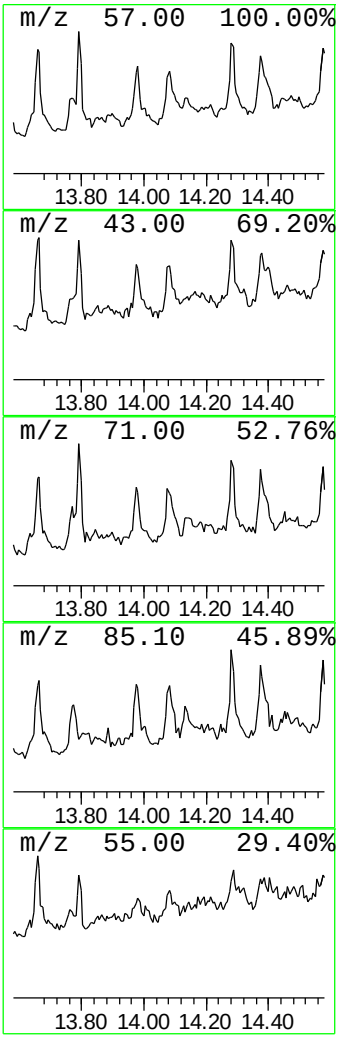
****

Peak Number 8 Sulfurous acid, 2-propyl tr... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.08	2.05 ng	151744	Chrysene-d12	13.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	87
2	2-methylhexacosane	380	C27H56	1000376-72-7	83
3	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	83
4	Behenyl chloride	344	C22H45Cl	042217-03-8	81
5	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	80





Library Search Compound Report

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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-10-10.5-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

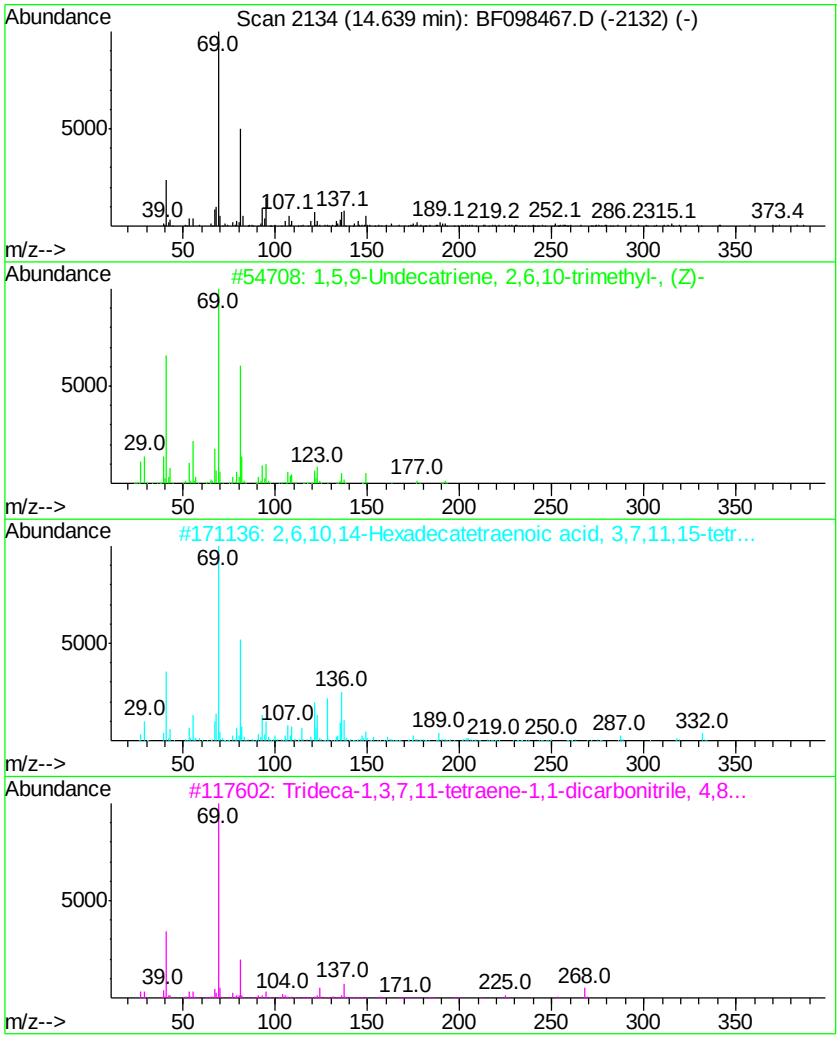
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

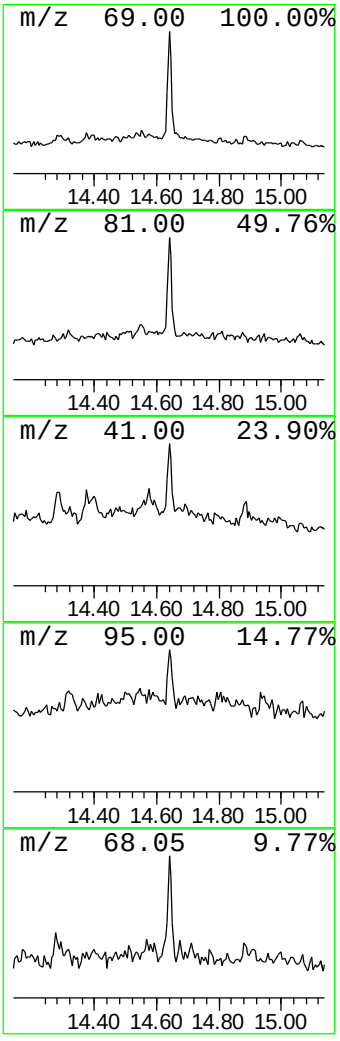
****

Peak Number 9 1,5,9-Undecatriene, 2,6,10-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	3.04 ng	146803	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	83
2	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64
3	Trideca-1,3,7,11-tetraene-1,1-di...	268	C18H24N2	1000159-88-9	59
4	Supraene	410	C30H50	007683-64-9	56
5	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	53





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Data File : BF098467.D
Acq On : 12 Sep 2017 23:06
Operator : SJ/JU
Sample : I5140-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-10-10.5-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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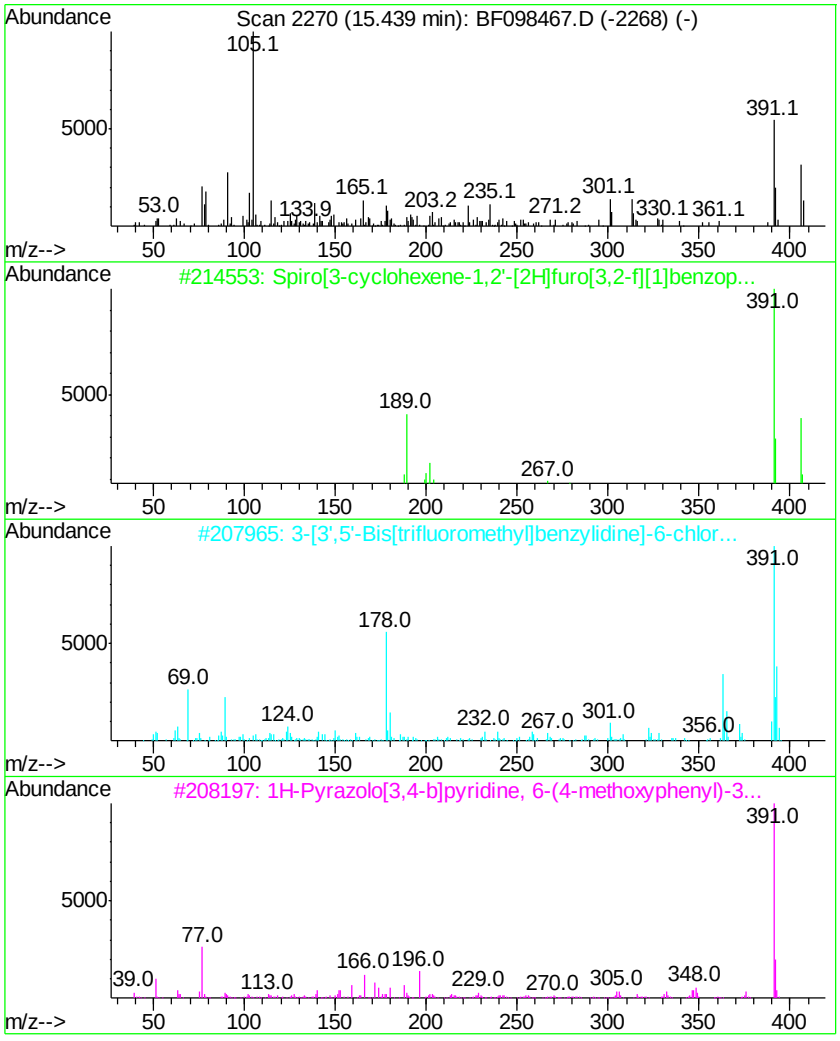
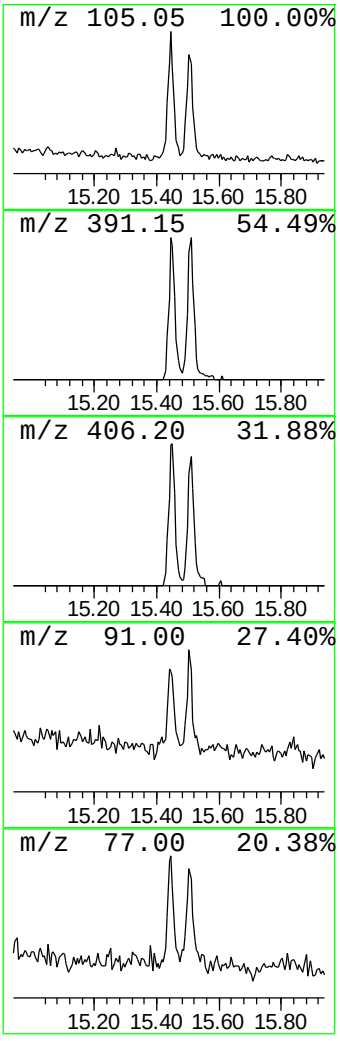
Peak Number 10 unknown15.44 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.44	4.17 ng	201067	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Spiro[3-cyclohexene-1,2'-[2H]fur...	406	C26H30O4	031642-63-4	36
2	3-[3',5'-Bis[trifluoromethyl]ben...	391	C17H8ClF6NO	1000252-19-8	27
3	1H-Pyrazolo[3,4-b]pyridine, 6-(4...	391	C26H21N3O	1000310-98-6	22
4	Silane, dimethyl(1-phenylpropoxy...	420	C26H48O2Si	1000347-28-3	16
5	Silane, diethyl(2-phenylethoxy)t...	420	C26H48O2Si	1000363-16-9	16





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF091217\
Data File : BF098467.D
Acq On : 12 Sep 2017 23:06
Operator : SJ/JU
Sample : I5140-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-10-10.5-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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
2-Pentanone, 4-hy...	4.85	8.2	ng	548161	1	6.66	1342260	20.0
unknown6.44	6.44	76.7	ng	5146330	1	6.66	1342260	20.0
Tridecane	10.60	2.3	ng	150923	4	11.17	1313410	20.0
Cycloeicosane	13.66	2.8	ng	209330	5	13.81	1477610	20.0
Cholest-14-en-3-o...	13.71	3.8	ng	277451	5	13.81	1477610	20.0
Sulfurous acid, 2...	14.08	2.0	ng	151744	5	13.81	1477610	20.0
1,5,9-Undecatrien...	14.64	3.0	ng	146803	6	15.21	964419	20.0
unknown15.44	15.44	4.2	ng	201067	6	15.21	964419	20.0