LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098588.D
Acq On : 16 Sep 2017 00:18
Operator : SJ/JU
Sample : I5123-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-06

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	4.822	462	465	478	rBV	258512	375454	10.42%	1.145%
2	5.257	534	539	558	rBV	2821534	3016178	83.73%	9.196%
3	6.298	712	716	727	rBV	2872070	3133515	86.98%	9.553%
4	6.416	732	736	739	rBV	3326134	3051963	84.72%	9.305%
5	6.639	771	774	780	rVB	818775	793203	22.02%	2.418%
6	6.798	797	801	812	rBV	2628917	2321015	64.43%	7.076%
7	7.216	867	872	875	rBV	2007659	1819030	50.49%	5.546%
8	7.928	987	993	996	rBV	1262388	1066743	29.61%	3.252%
9	7.992	1002	1004	1007	rVB	97826	73902	2.05%	0.225%
10	8.216	1038	1042	1045	rVB5	28575	41238	1.14%	0.126%
11	8.351	1061	1065	1071	rBV	105973	137921	3.83%	0.420%
12	8.622	1107	1111	1114	rVB2	57074	71192	1.98%	0.217%
13	8.745	1129	1132	1137	rVB3	36136	51849	1.44%	0.158%
14	8.833	1144	1147	1151	rVB4	34952	40550	1.13%	0.124%
15	8.875	1151	1154	1156	rBV3	40620	44850	1.24%	0.137%
16	8.951	1162	1167	1171	rBV	168960	160310	4.45%	0.489%
17	9.004	1171	1176	1179	rBV	3735037	3602469	100.00%	10.983%
18	9.086	1185	1190	1194	rBV6	52047	100069	2.78%	0.305%
19	9.275	1218	1222	1224	rVB2	45347	47693	1.32%	0.145%
20	9.339	1230	1233	1235	rBV	62638	56556	1.57%	0.172%
21	9.404	1241	1244	1247	rVB	536570	435465	12.09%	1.328%
22	9.457	1251	1253	1257	rVB3	35523	41513	1.15%	0.127%
23	9.539	1265	1267	1272	rBV4	31315	39632	1.10%	0.121%
24	9.616	1278	1280	1284	rVB3	44646	40994	1.14%	0.125%
25	9.680	1284	1291	1294	rBV	1314559	1237484	34.35%	3.773%
26	9.786	1306	1309	1312	rVB2	51272	58779	1.63%	0.179%
27	9.833	1314	1317	1320	rBV5	26154	43942	1.22%	0.134%
28	9.880	1322	1325	1330	rVV3	84131	105443	2.93%	0.321%
29	9.939	1333	1335	1338	rVV3	65019	57741	1.60%	0.176%
30	9.998	1342	1345	1348	rBV4	48581	56144	1.56%	0.171%
31	10.086	1357	1360	1362	rBV	46064	56963	1.58%	0.174%
32	10.110	1362	1364	1367	rVB2	50903	56124	1.56%	0.171%
33	10.222	1379	1383	1385	rBV3	36862	52495	1.46%	0.160%
34	10.333	1396	1402	1407	rBV	191806	225446	6.26%	0.687%

LSC Area Percent Report

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Data File : BF098588.D
Acq On : 16 Sep 2017 00:18
Operator : SJ/JU
Sample : I5123-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-06

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	10.380	1408	1410	1414	rVB4	34169	45924	1.27%	0.140%
36	10.469	1419	1425	1429	rBV	1810516	1724593	47.87%	5.258%
37	10.545	1436	1438	1442	rBV5	38541	55928	1.55%	0.171%
38	10.598	1442	1447	1453	rVB	339499	399856	11.10%	1.219%
39	10.922	1498	1502	1504	rBV4	34312	53864	1.50%	0.164%
40	11.033	1518	1521	1523	rBV	58311	49035	1.36%	0.149%
41	11.063	1523	1526	1532	rVB	224229	234491	6.51%	0.715%
42	11.163	1539	1543	1545	rBV	1233411	1072350	29.77%	3.269%
43	11.186	1545	1547	1550	rVB	164969	139004	3.86%	0.424%
44	11.410	1580	1585	1589	rVB4	53928	88358	2.45%	0.269%
45	11.663	1625	1628	1631	rBV	63678	58911	1.64%	0.180%
46	11.692	1631	1633	1636	rVB	83055	63937	1.77%	0.195%
47	11.774	1644	1647	1649	rBV2	70327	73795	2.05%	0.225%
48	11.798	1649	1651	1655	rVB	61416	54374	1.51%	0.166%
49	12.139	1706	1709	1716	rBV5	55605	86150	2.39%	0.263%
50	12.210	1718	1721	1724	rVV	68702	63790	1.77%	0.194%
51	12.251	1725	1728	1733	rVB5	49448	74691	2.07%	0.228%
52	12.374	1746	1749	1754	rVB	143731	134475	3.73%	0.410%
53	12.598	1784	1787	1790	rBV	140072	133510	3.71%	0.407%
54	12.651	1794	1796	1800	rVB2	54567	54823	1.52%	0.167%
55	12.751	1808	1813	1816	rBV	2516514	2524752	70.08%	7.697%
56	13.033	1859	1861	1868	rVB5	38956	52702	1.46%	0.161%
57	13.321	1906	1910	1912	rBV4	43308	57095	1.58%	0.174%
58	13.439	1927	1930	1934	rBV2	75523	74209	2.06%	0.226%
59	13.645	1962	1965	1971	rBV2	281644	344611	9.57%	1.051%
60	13.698	1971	1974	1979	rVB	169183	160729	4.46%	0.490%
61	13.798	1985	1991	1994	rBV2	853047	1003761	27.86%	3.060%
62	14.068	2034	2037	2044	rVB7	44847	95066	2.64%	0.290%
63	14.280	2069	2073	2080	rVB3	84946	168112	4.67%	0.513%
64	14.362	2085	2087	2090	rBV2	43786	63233	1.76%	0.193%
65	14.627	2130	2132	2135	rVB	88968	74183	2.06%	0.226%
66	15.198	2225	2229	2239	rBV	556273	723213	20.08%	2.205%
67	15.427	2265	2268	2273	rVB2	70037	84634	2.35%	0.258%
68	15.486	2275	2278	2283	rVB5	84417	126103	3.50%	0.384%
69	15.656	2303	2307	2314	rVB5	38827	72102	2.00%	0.220%

Sum of corrected areas: 32800229

LSC Report - Integrated Chromatogram

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Data File : BF098588.D
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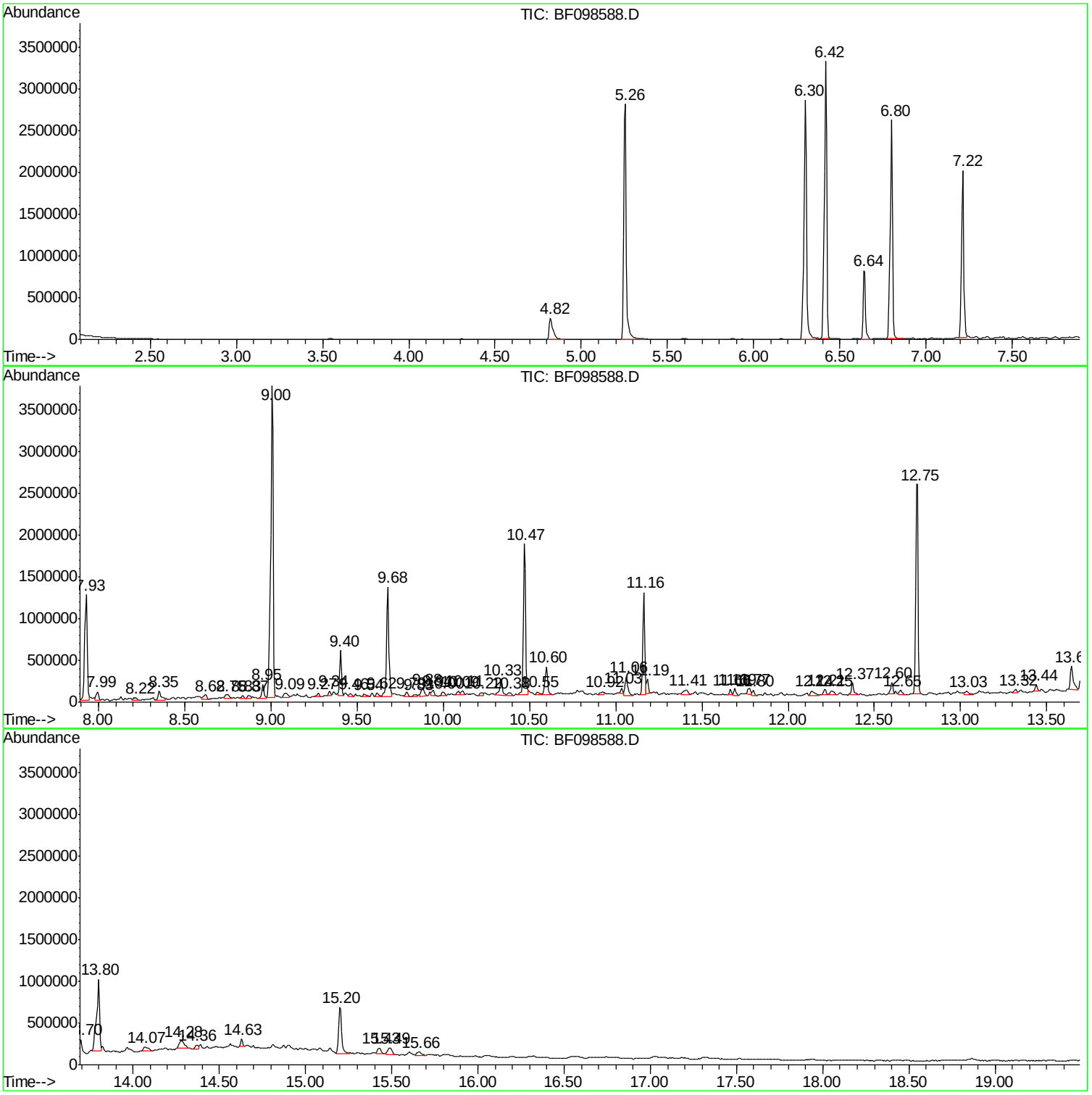
Operator : SJ/JU
Sample : I5123-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-06

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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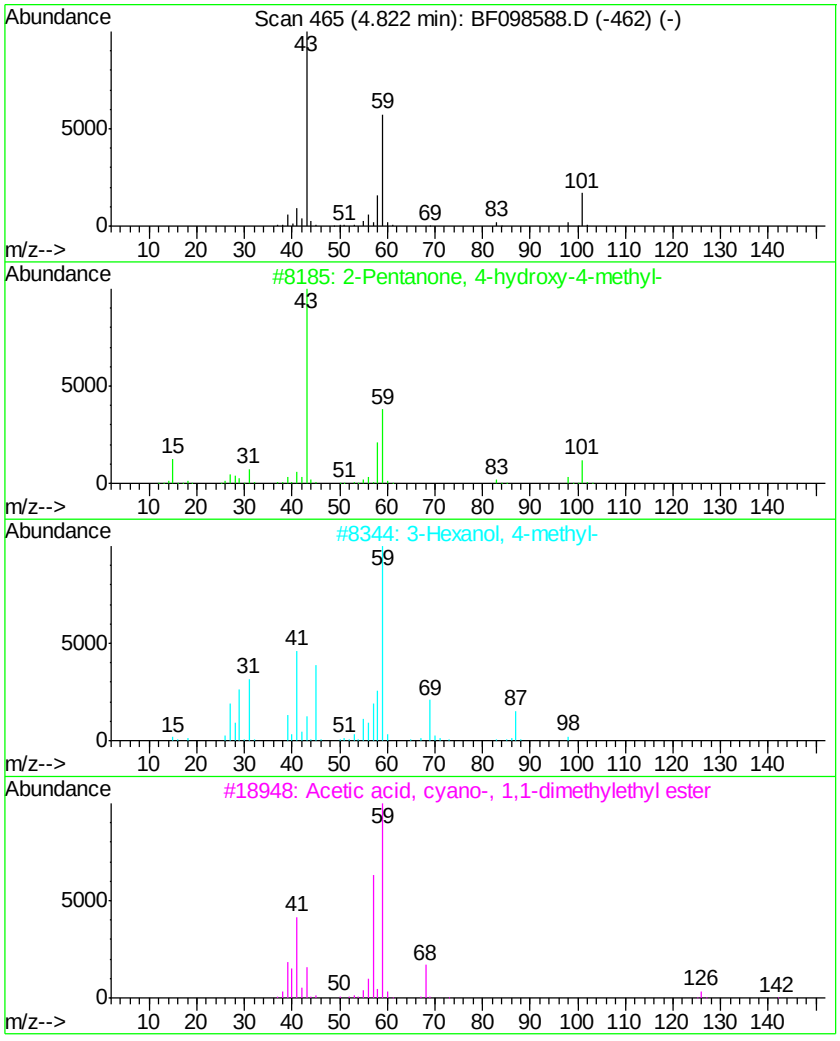
TIC Integration Parameters: LSCINT.P

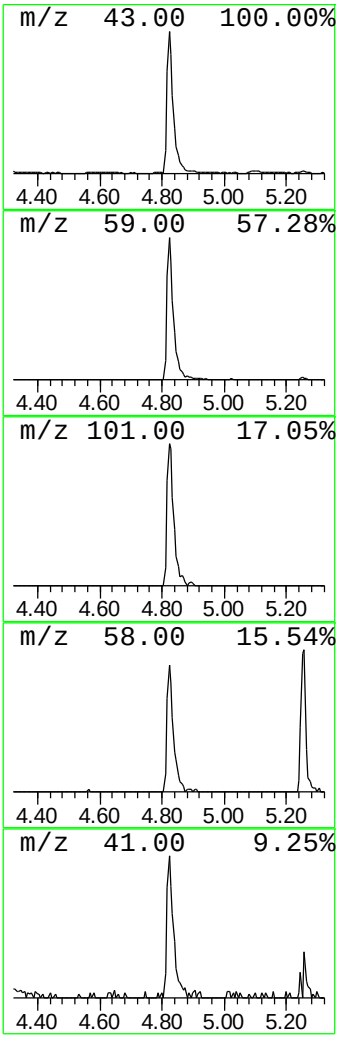
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	9.47 ng	375454	1,4-Dichlorobenzene-d4	6.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	4-Methoxy-1-pentene	100	C6H12O	098386-09-5	23





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098588.D
Acq On : 16 Sep 2017 00:18
Operator : SJ/JU
Sample : I5123-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-06

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

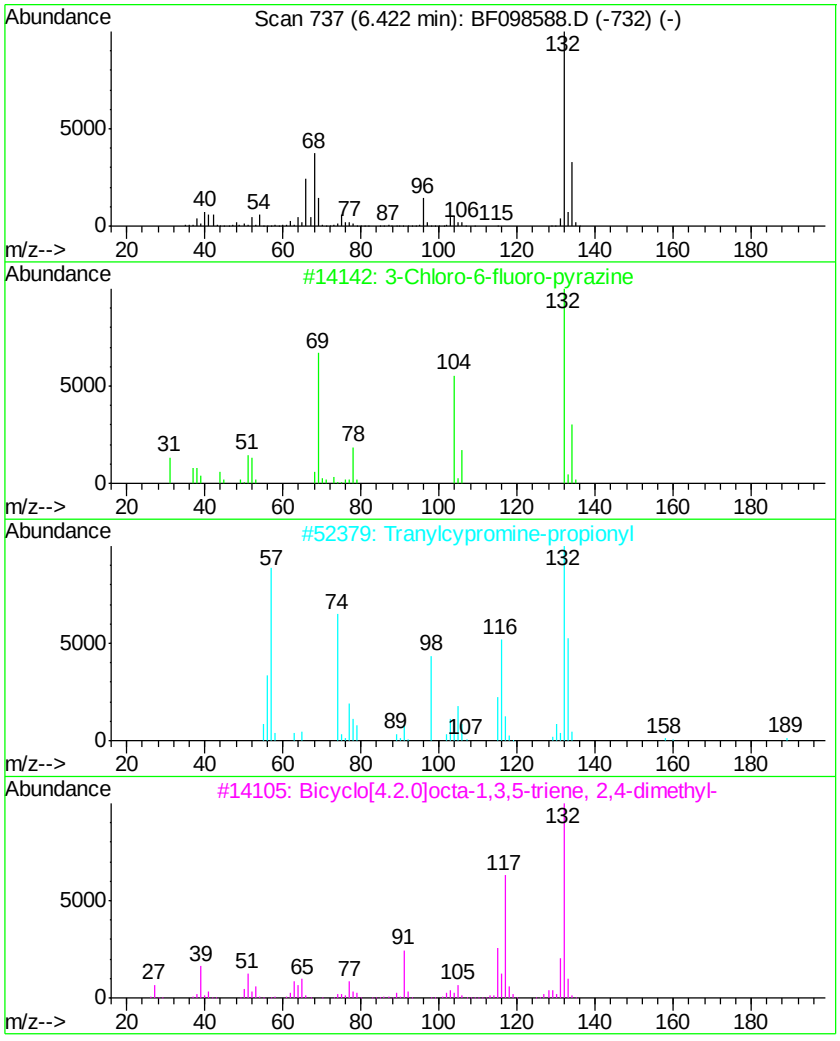
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

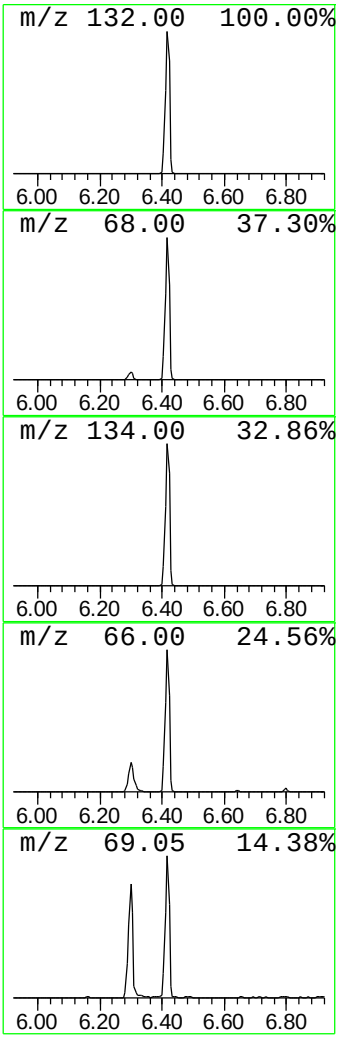
****

Peak Number 2 unknown6.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	76.95 ng	3051960	1,4-Dichlorobenzene-d4	6.65

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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098588.D
Acq On : 16 Sep 2017 00:18
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Sample : I5123-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-06

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

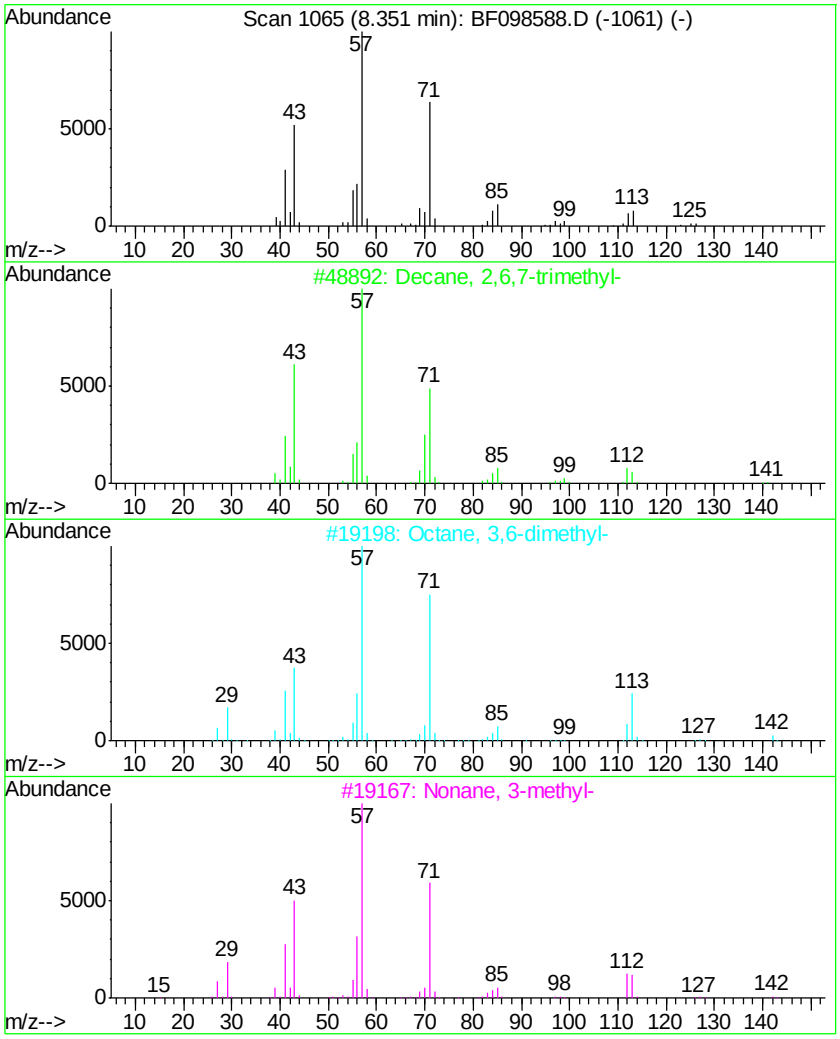
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

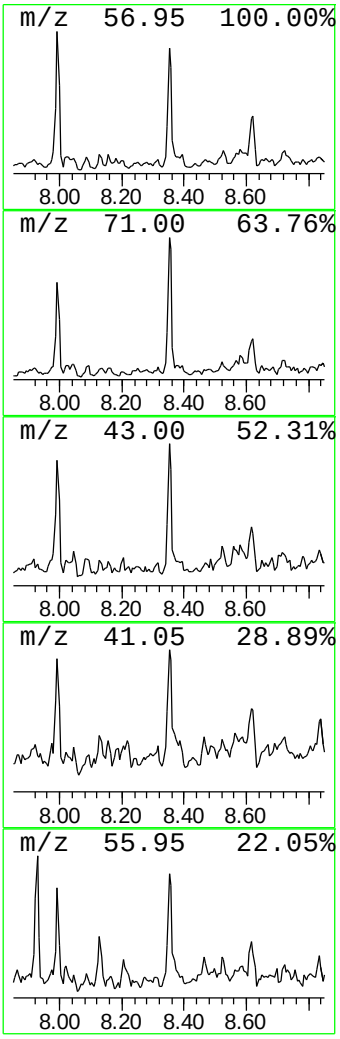
****

Peak Number 4 Decane, 2,6,7-trimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.35	2.59 ng	137921	Naphthalene-d8	7.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	90
2	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	78
3	Nonane, 3-methyl-	142	C10H22	005911-04-6	78
4	Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	72
5	Sulfurous acid, butyl 2-ethylhex...	250	C12H26O3S	1000309-18-8	64





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
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Sample : I5123-01
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Instrument : BNA_F
ClientSampleId : EP-06

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
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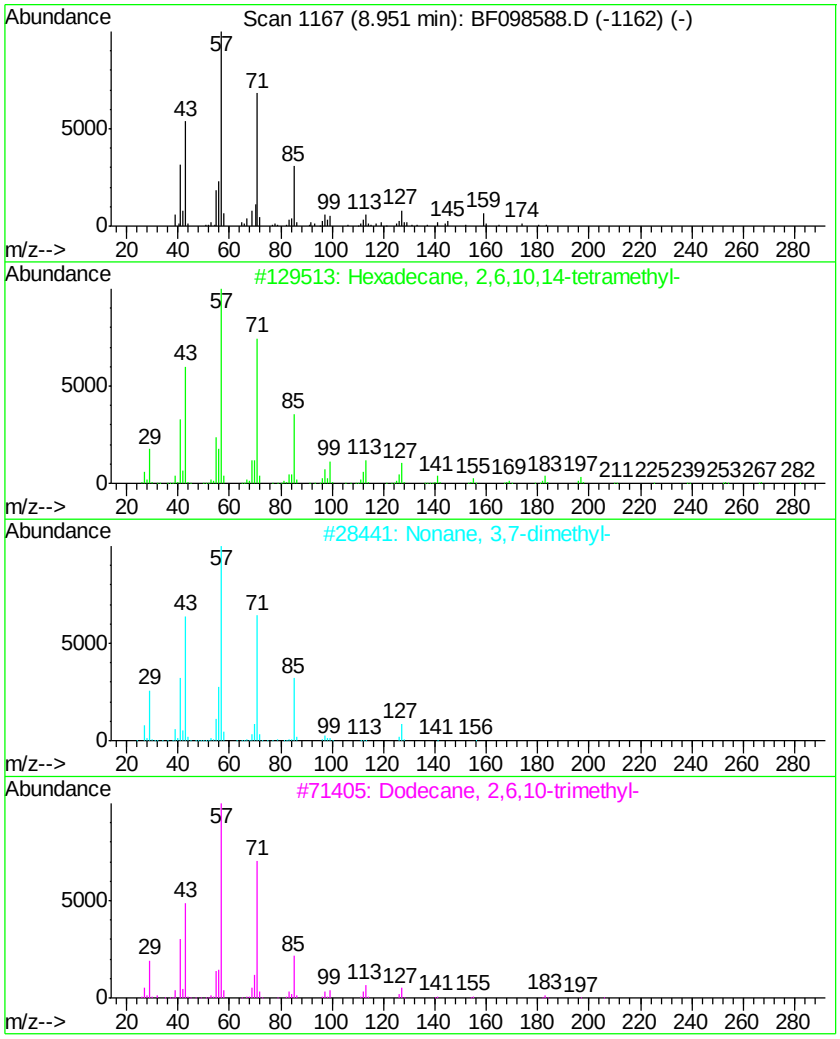
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

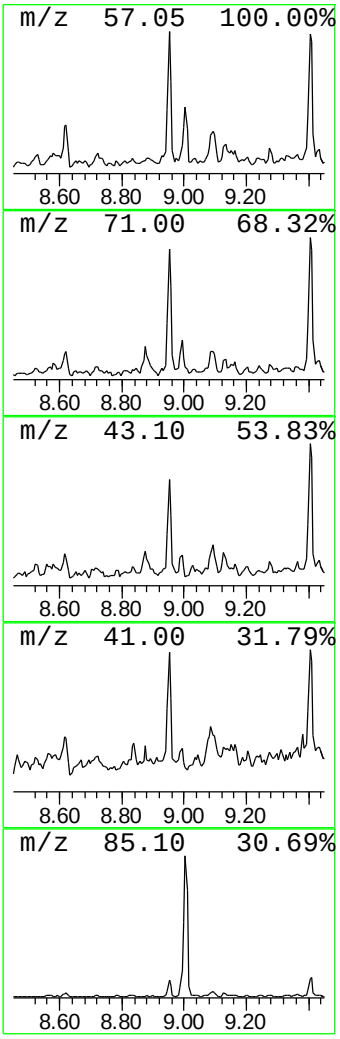
****

Peak Number 5 Hexadecane, 2,6,10,14-tetra... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.95	2.59 ng	160310	Acenaphthene-d10	9.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	72
2	Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	72
3	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	64
4	Hexadecane	226	C16H34	000544-76-3	64
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	59





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Instrument : BNA_F
ClientSampleId : EP-06

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
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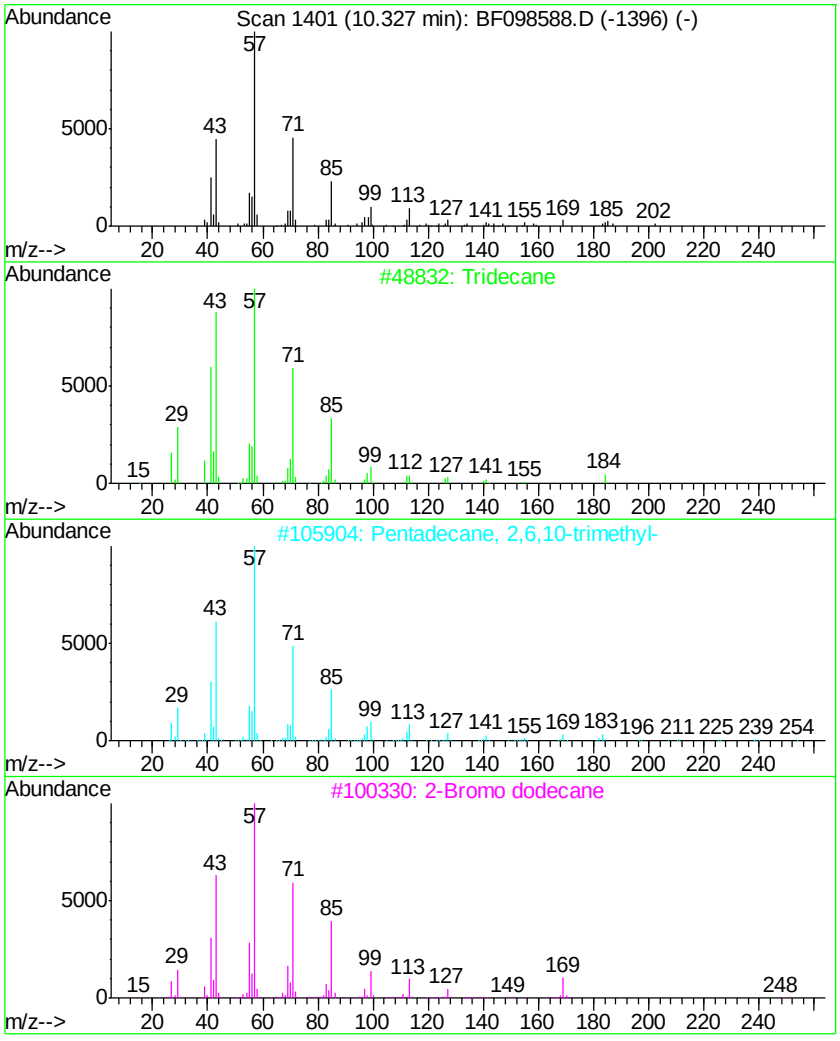
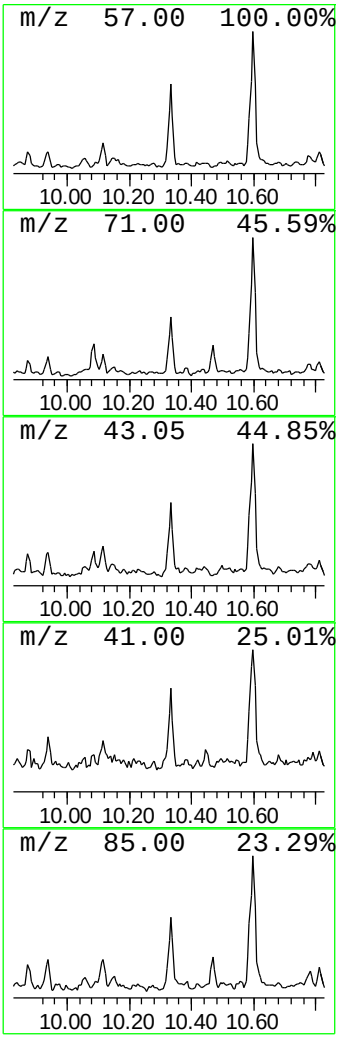
****

Peak Number 6 Tridecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.33	3.64 ng	225446	Acenaphthene-d10	9.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	87
2	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	80
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	72
4	Heneicosane	296	C21H44	000629-94-7	72
5	Tetradecane	198	C14H30	000629-59-4	64





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Sample : I5123-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-06

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

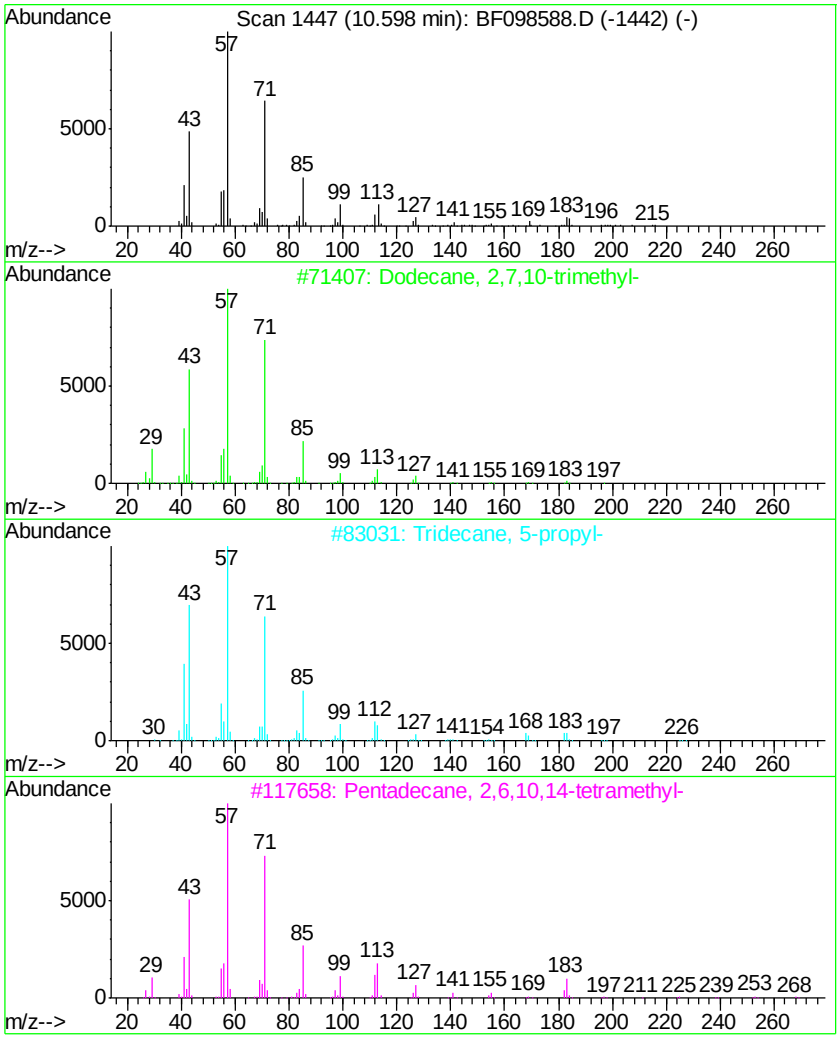
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

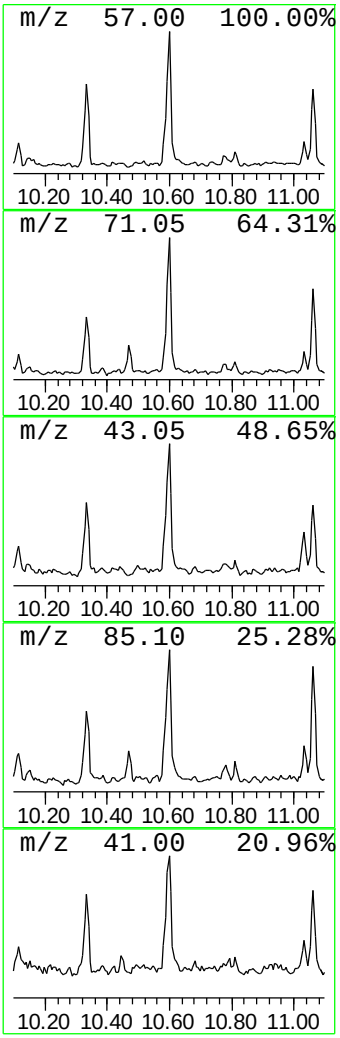
****

Peak Number 7 Dodecane, 2,7,10-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	7.46 ng	399856	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	80
2	Tridecane, 5-propyl-	226	C16H34	055045-11-9	78
3	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	72
4	5,5-Dibutylnonane	240	C17H36	006008-17-9	64
5	Tridecane, 3-methyl-	198	C14H30	006418-41-3	62





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098588.D
Acq On : 16 Sep 2017 00:18
Operator : SJ/JU
Sample : I5123-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-06

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

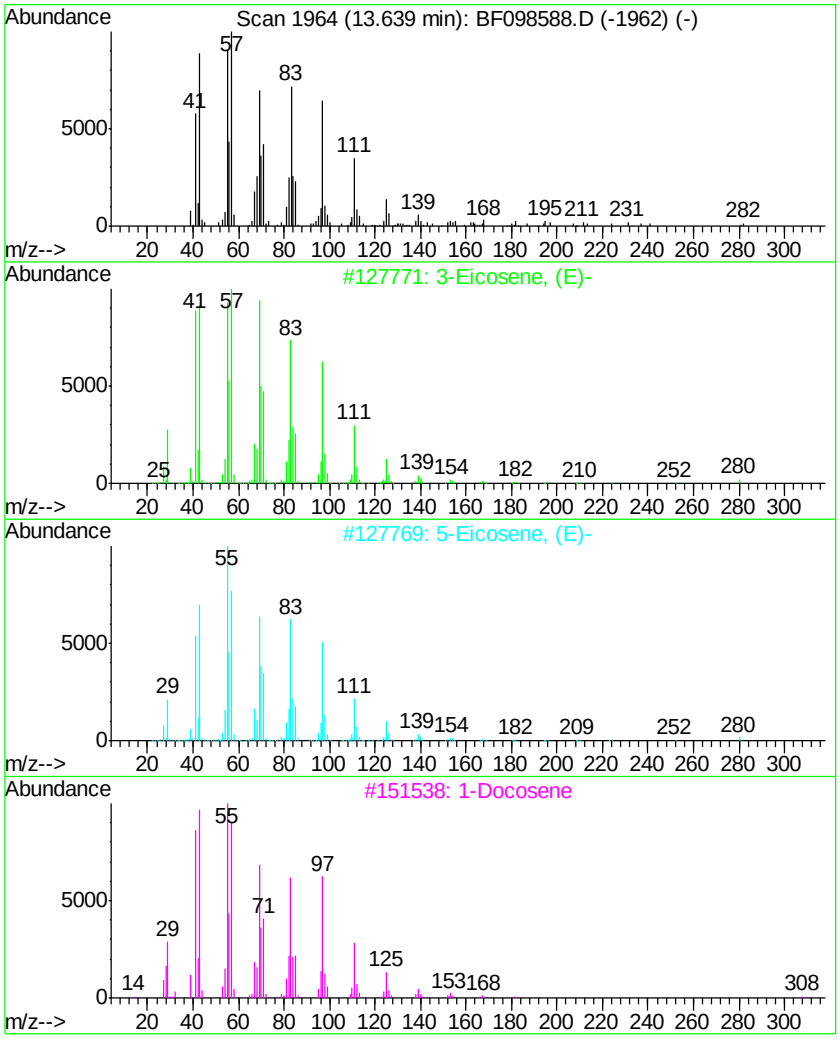
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

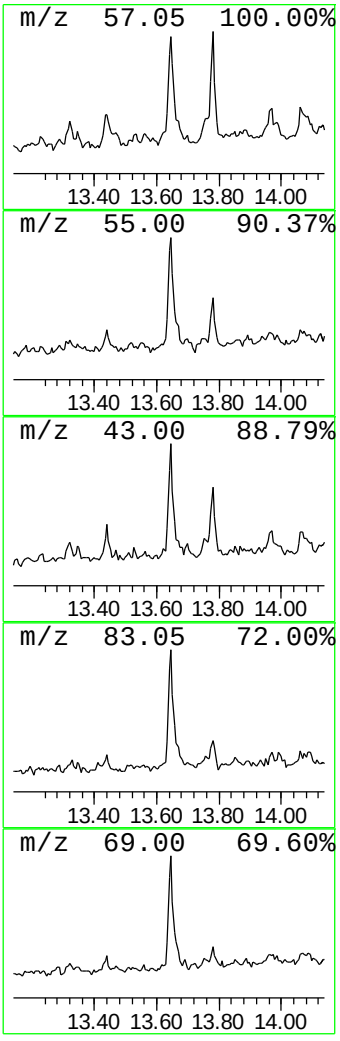
****

Peak Number 9 3-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.64	6.87 ng	344611	Chrysene-d12	13.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	96
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	96
3	1-Docosene	308	C22H44	001599-67-3	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94





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Acq On : 16 Sep 2017 00:18
Operator : SJ/JU
Sample : I5123-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-06

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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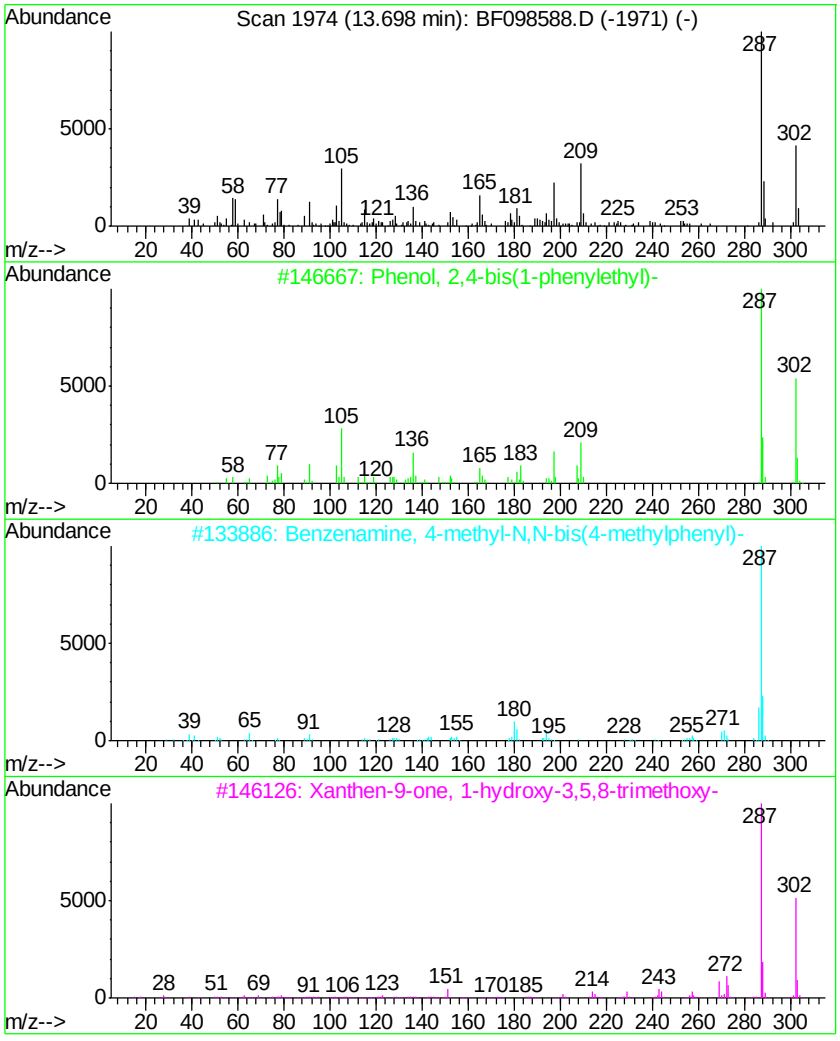
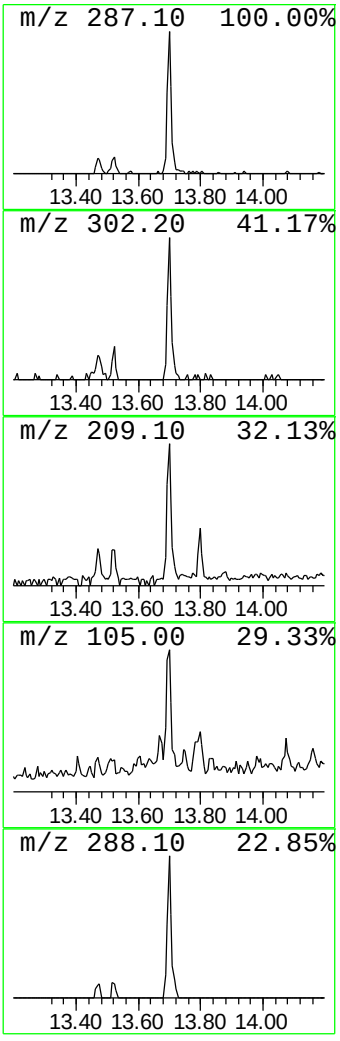
Peak Number 10 Phenol, 2,4-bis(1-phenyleth... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	3.20 ng	160729	Chrysene-d12	13.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,4-bis(1-phenylethyl)-	302	C22H22O	002769-94-0	94
2	Benzenamine, 4-methyl-N,N-bis(4-...	287	C21H21N	1000327-28-1	50
3	Xanthen-9-one, 1-hydroxy-3,5,8-t...	302	C16H14O6	049599-09-9	50
4	p-Methoxybenzylidene p-biphenyla...	287	C20H17NO	025543-63-9	43
5	Silane, diethyldiheptyloxy-	316	C18H40O2Si	1000363-95-3	35





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Operator : SJ/JU
Sample : I5123-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-06

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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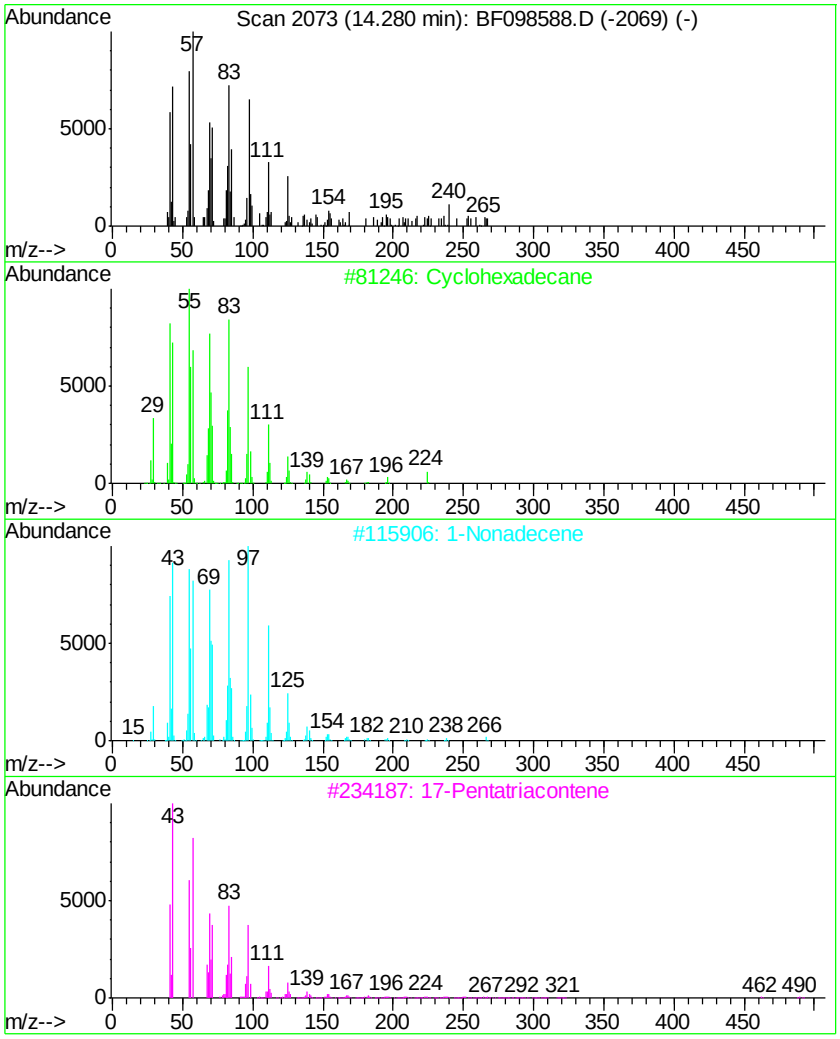
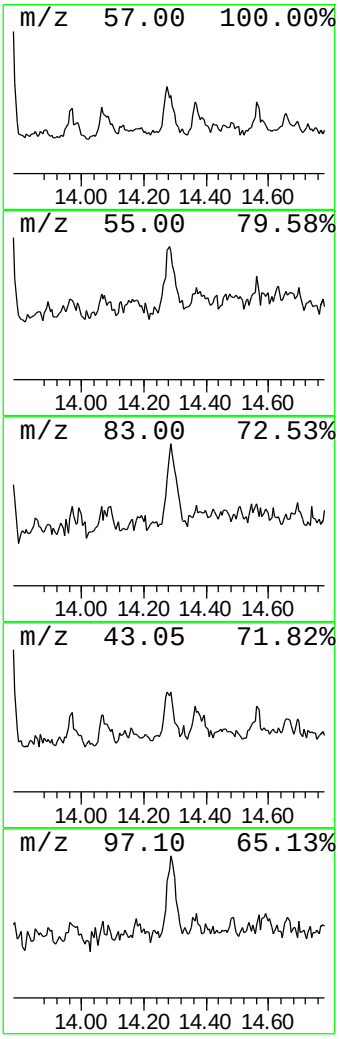
Peak Number 11 Cyclohexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.28	3.35 ng	168112	Chrysene-d12	13.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	86
2	1-Nonadecene	266	C19H38	018435-45-5	86
3	17-Pentatriacontene	491	C35H70	006971-40-0	74
4	Cyclopentadecane	210	C15H30	000295-48-7	70
5	1-Octadecene	252	C18H36	000112-88-9	70





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Sample : I5123-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-06

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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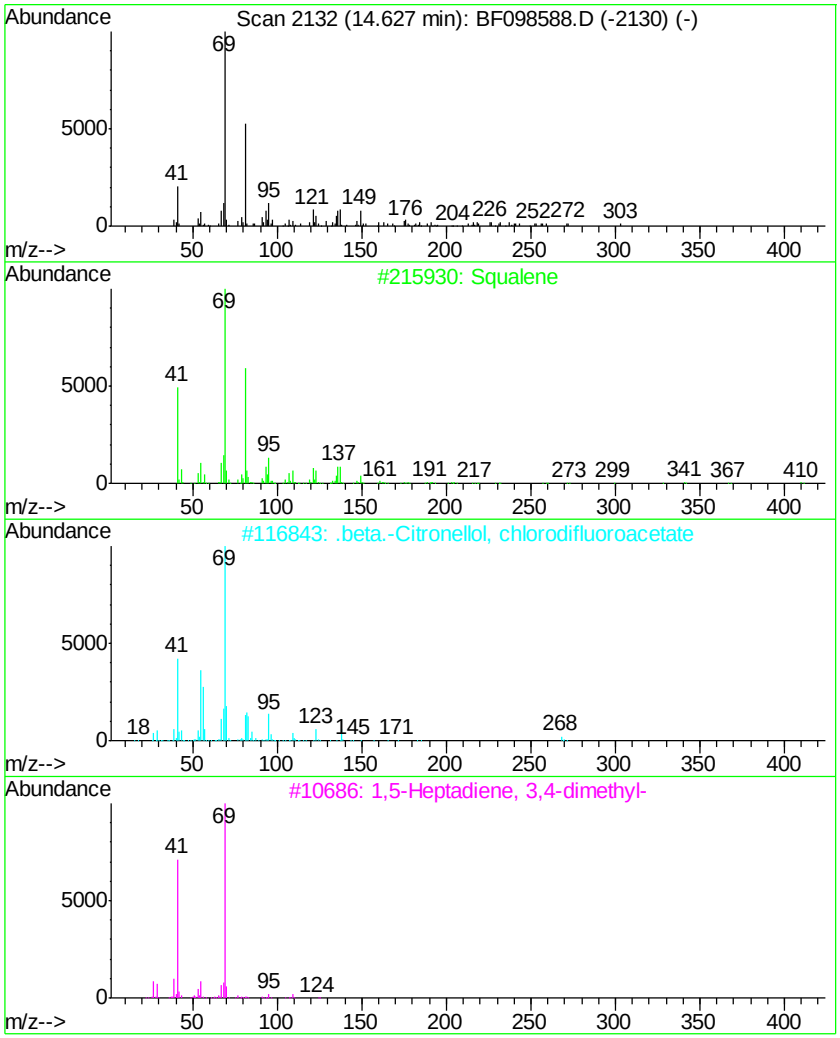
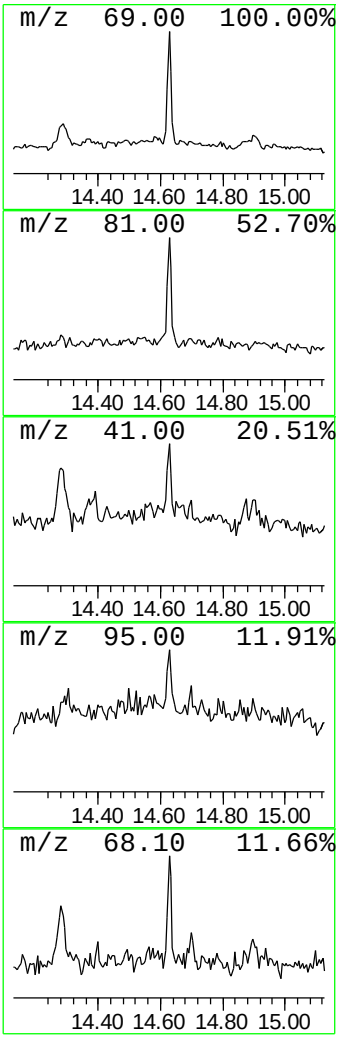
Peak Number 12 Squalene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	2.05 ng	74183	Perylene-d12	15.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	72
2	.beta.-Citronellol, chlorodifluo...	268	C12H19ClF2O2	1000376-20-8	64
3	1,5-Heptadiene, 3,4-dimethyl-	124	C9H16	1000061-77-9	59
4	trans-Farnesol	222	C15H26O	000106-28-5	50
5	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50





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Sample : I5123-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-06

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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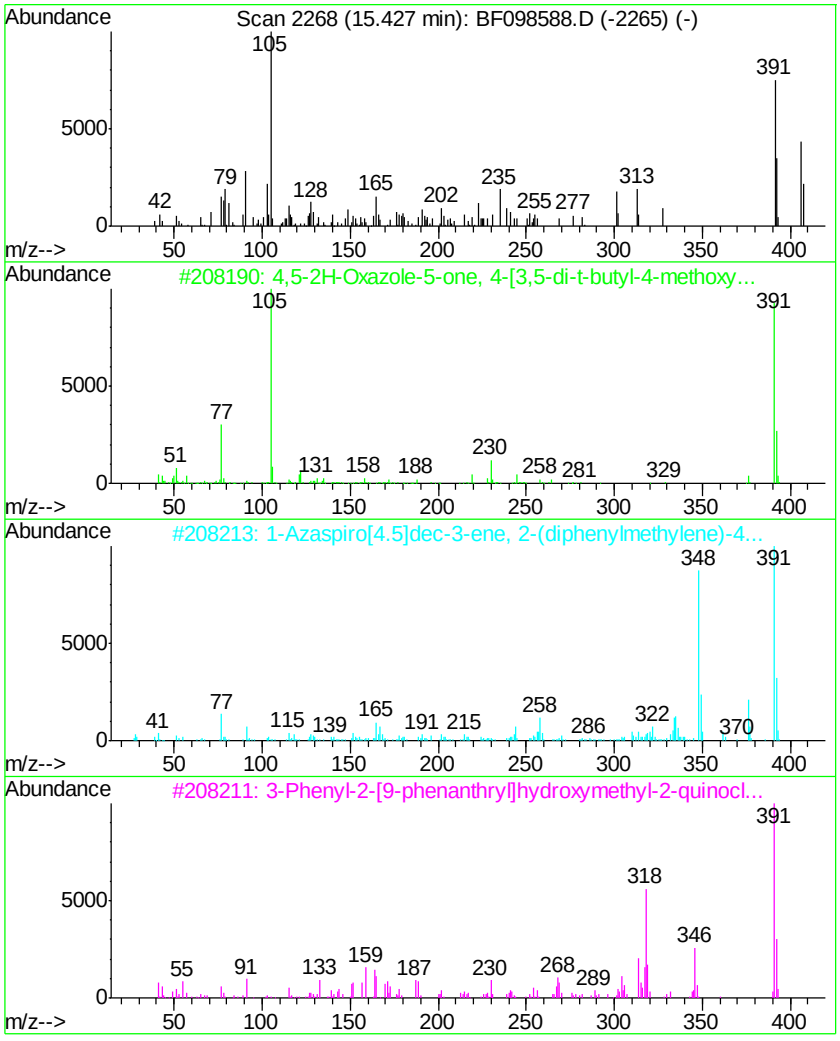
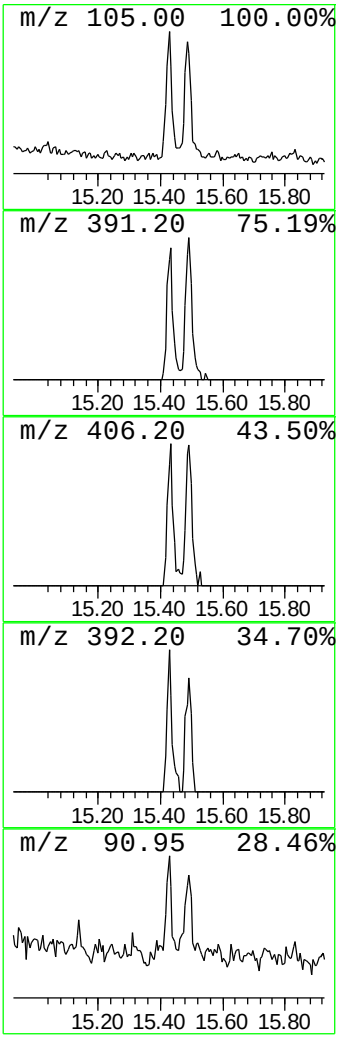
Peak Number 13 unknown15.43 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.43	2.34 ng	84634	Perylene-d12	15.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,5-2H-Oxazole-5-one, 4-[3,5-di-...	391	C25H29NO3	1000130-25-1	38
2	1-Azaspiro[4.5]dec-3-ene, 2-(dip...	391	C29H29N	100942-44-7	35
3	3-Phenyl-2-[9-phenanthryl]hydrox...	391	C28H25NO	1000252-87-9	25
4	Benzoic acid, 3-heptafluorobutyr...	448	C17H19F7O4Si	1000375-03-0	16
5	1H-Dicyclooct[e,g]isoindole-1,3(...	391	C26H33NO2	051624-51-2	16





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Acq On : 16 Sep 2017 00:18
Operator : SJ/JU
Sample : I5123-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-06

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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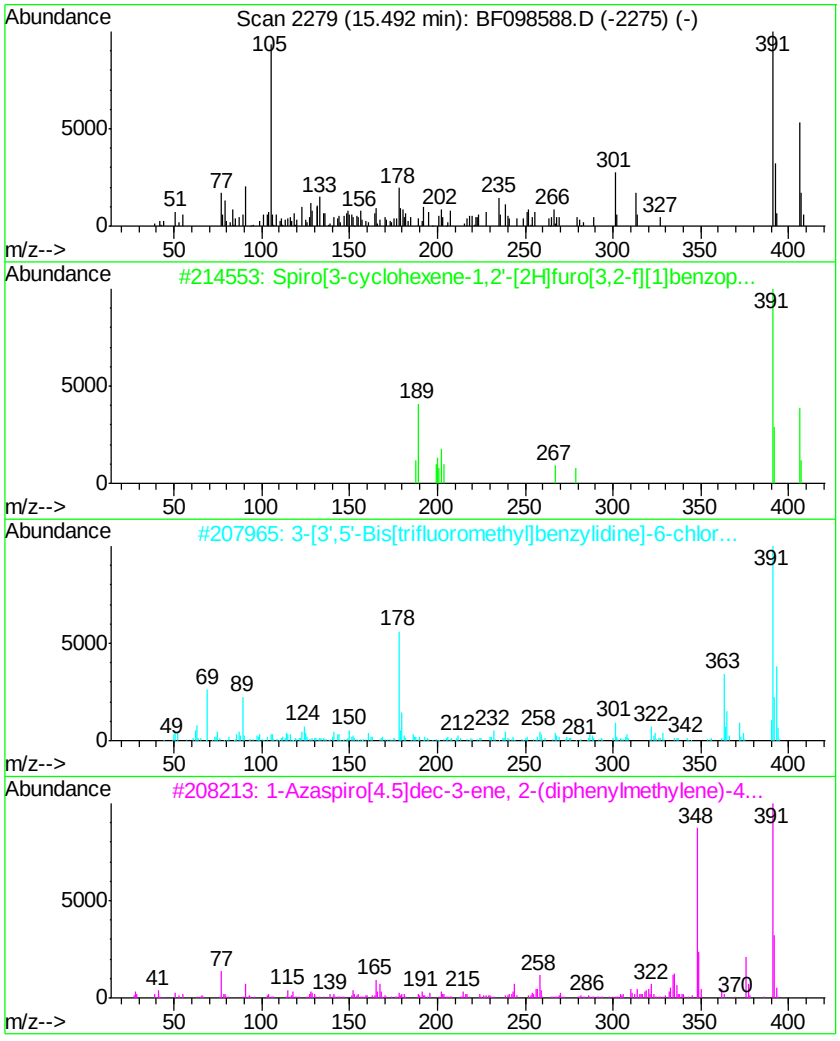
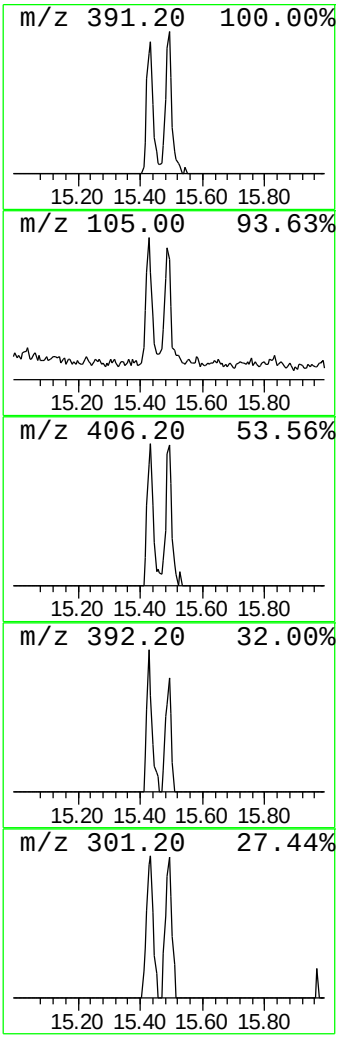
Peak Number 14 Spiro[3-cyclohexene-1,2'-[2... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.49	3.49 ng	126103	Perylene-d12	15.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Spiro[3-cyclohexene-1,2'-[2H]fur...	406	C26H30O4	031642-63-4	53
2	3-[3',5'-Bis[trifluoromethyl]ben...	391	C17H8ClF6NO	1000252-19-8	38
3	1-Azaspiro[4.5]dec-3-ene, 2-(dip...	391	C29H29N	100942-44-7	38
4	4,5-2H-Oxazole-5-one, 4-[3,5-di-...	391	C25H29NO3	1000130-25-1	35
5	Piperazinetrione, [[2-(1,1-dimet...	391	C23H25N3O3	025644-25-1	35





Tentatively Identified Compound (LSC) summary

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Operator : SJ/JU
Sample : I5123-01
Misc :
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Instrument : BNA_F
ClientSampleId : EP-06

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...	4.82	9.5	ng	375454	1	6.65	793203	20.0
unknown6.42	6.42	77.0	ng	3051960	1	6.65	793203	20.0
Decane, 2,6,7-tri...	8.35	2.6	ng	137921	2	7.93	1066740	20.0
Hexadecane, 2,6,1...	8.95	2.6	ng	160310	3	9.68	1237480	20.0
Tridecane	10.33	3.6	ng	225446	3	9.68	1237480	20.0
Dodecane, 2,7,10-...	10.60	7.5	ng	399856	4	11.16	1072350	20.0
3-Eicosene, (E)-	13.64	6.9	ng	344611	5	13.80	1003760	20.0
Phenol, 2,4-bis(1...	13.70	3.2	ng	160729	5	13.80	1003760	20.0
Cyclohexadecane	14.28	3.4	ng	168112	5	13.80	1003760	20.0
Squalene	14.63	2.0	ng	74183	6	15.20	723213	20.0
unknown15.43	15.43	2.3	ng	84634	6	15.20	723213	20.0
Spiro[3-cyclohexe...	15.49	3.5	ng	126103	6	15.20	723213	20.0