LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092717\
Data File : BF098883.D
Acq On : 28 Sep 2017 00:48
Operator : SJ/JU
Sample : I5249-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF1

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-BF092317.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	2.216	17	22	30	rVB	97956	126592	3.70%	0.387%
2	5.145	516	520	530	rVB	491313	626478	18.33%	1.915%
3	5.539	581	587	590	rBV	3259652	3289028	96.24%	10.055%
4	6.539	752	757	770	rVB	2849766	3417625	100.00%	10.448%
5	6.686	777	782	785	rBV	3491647	3318364	97.10%	10.145%
6	6.916	816	821	824	rBV	1013726	827889	24.22%	2.531%
7	6.969	826	830	833	rVB	61764	46686	1.37%	0.143%
8	7.075	844	848	851	rBV	2439464	2228590	65.21%	6.813%
9	7.475	911	916	919	rBV	1975133	1999278	58.50%	6.112%
10	8.198	1035	1039	1041	rBV	1179017	1079870	31.60%	3.301%
11	8.216	1041	1042	1045	rVB	530879	357369	10.46%	1.093%
12	8.827	1142	1146	1150	rBV	129265	121093	3.54%	0.370%
13	8.910	1157	1160	1162	rVB	53929	46119	1.35%	0.141%
14	9.269	1216	1221	1224	rBV	3007637	2697994	78.94%	8.248%
15	9.663	1284	1288	1296	rVB	565736	519429	15.20%	1.588%
16	9.810	1310	1313	1316	rBV	67201	61670	1.80%	0.189%
17	9.874	1319	1324	1327	rVV	36676	39885	1.17%	0.122%
18	9.951	1331	1337	1341	rVV	1096685	980791	28.70%	2.998%
19	9.986	1341	1343	1346	rVB	56369	43511	1.27%	0.133%
20	10.151	1366	1371	1375	rVB3	42644	54432	1.59%	0.166%
21	10.351	1402	1405	1407	rBV2	34709	47481	1.39%	0.145%
22	10.374	1407	1409	1412	rVB	66792	50658	1.48%	0.155%
23	10.498	1427	1430	1432	rBV2	49593	42417	1.24%	0.130%
24	10.592	1442	1446	1448	rBV	43502	51052	1.49%	0.156%
25	10.739	1467	1471	1475	rVB	1648208	1489410	43.58%	4.553%
26	10.863	1486	1492	1498	rVB5	119036	195444	5.72%	0.597%
27	10.916	1498	1501	1503	rBV	37757	37917	1.11%	0.116%
28	11.045	1518	1523	1525	rBV6	33960	58255	1.70%	0.178%
29	11.092	1529	1531	1535	rVB4	38315	44943	1.32%	0.137%
30	11.292	1562	1565	1567	rBV2	53503	49230	1.44%	0.151%
31	11.327	1568	1571	1577	rVB3	54516	80886	2.37%	0.247%
32	11.439	1586	1590	1592	rBV	998668	844622	24.71%	2.582%
33	11.463	1592	1594	1596	rVV	279921	210875	6.17%	0.645%
34	11.516	1600	1603	1605	rVB	99123	79683	2.33%	0.244%

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Misc :
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Instrument : BNA_F
ClientSampleId : ROLL-OFF1

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

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Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.545	1605	1608	1611	rBV4	26655	37673	1.10%	0.115%
36	11.598	1614	1617	1622	rVB2	23421	36813	1.08%	0.113%
37	11.651	1622	1626	1628	rBV3	47136	70004	2.05%	0.214%
38	11.951	1672	1677	1679	rBV2	90774	139339	4.08%	0.426%
39	12.051	1691	1694	1697	rBV2	88397	97745	2.86%	0.299%
40	12.127	1705	1707	1712	rBV6	38219	41822	1.22%	0.128%
41	12.233	1723	1725	1727	rBV	44978	35582	1.04%	0.109%
42	12.410	1753	1755	1758	rBV2	37404	36983	1.08%	0.113%
43	12.486	1766	1768	1771	rBV	55608	56159	1.64%	0.172%
44	12.527	1771	1775	1777	rVV4	59196	77401	2.26%	0.237%
45	12.574	1780	1783	1787	rBV3	47916	44018	1.29%	0.135%
46	12.651	1793	1796	1800	rVB	516917	435984	12.76%	1.333%
47	12.692	1800	1803	1806	rBV4	50981	54825	1.60%	0.168%
48	12.745	1810	1812	1815	rVB	48287	42338	1.24%	0.129%
49	12.880	1829	1835	1842	rBV	472801	587919	17.20%	1.797%
50	12.933	1842	1844	1848	rVB2	43885	43555	1.27%	0.133%
51	13.021	1855	1859	1868	rVB	2170090	2036917	59.60%	6.227%
52	13.092	1869	1871	1876	rVV3	35445	51936	1.52%	0.159%
53	13.210	1888	1891	1895	rVB	107355	106958	3.13%	0.327%
54	13.274	1899	1902	1905	rBV	92553	82552	2.42%	0.252%
55	13.310	1906	1908	1911	rVB2	53833	54162	1.58%	0.166%
56	13.904	2006	2009	2018	rVB4	294213	336294	9.84%	1.028%
57	14.051	2031	2034	2035	rBV	241235	223877	6.55%	0.684%
58	14.080	2035	2039	2042	rVV2	927991	1068227	31.26%	3.266%
59	14.104	2042	2043	2050	rVB	257065	181638	5.31%	0.555%
60	14.539	2114	2117	2120	rBV2	70292	98481	2.88%	0.301%
61	14.921	2180	2182	2186	rBV	57258	55766	1.63%	0.170%
62	15.133	2214	2218	2221	rBV	162747	261235	7.64%	0.799%
63	15.439	2268	2270	2277	rVB	111150	155051	4.54%	0.474%
64	15.504	2278	2281	2288	rVV	147230	206089	6.03%	0.630%
65	15.574	2288	2293	2305	rVB	474792	726204	21.25%	2.220%
66	16.027	2368	2370	2375	rVB2	48305	61541	1.80%	0.188%

Sum of corrected areas: 32710654

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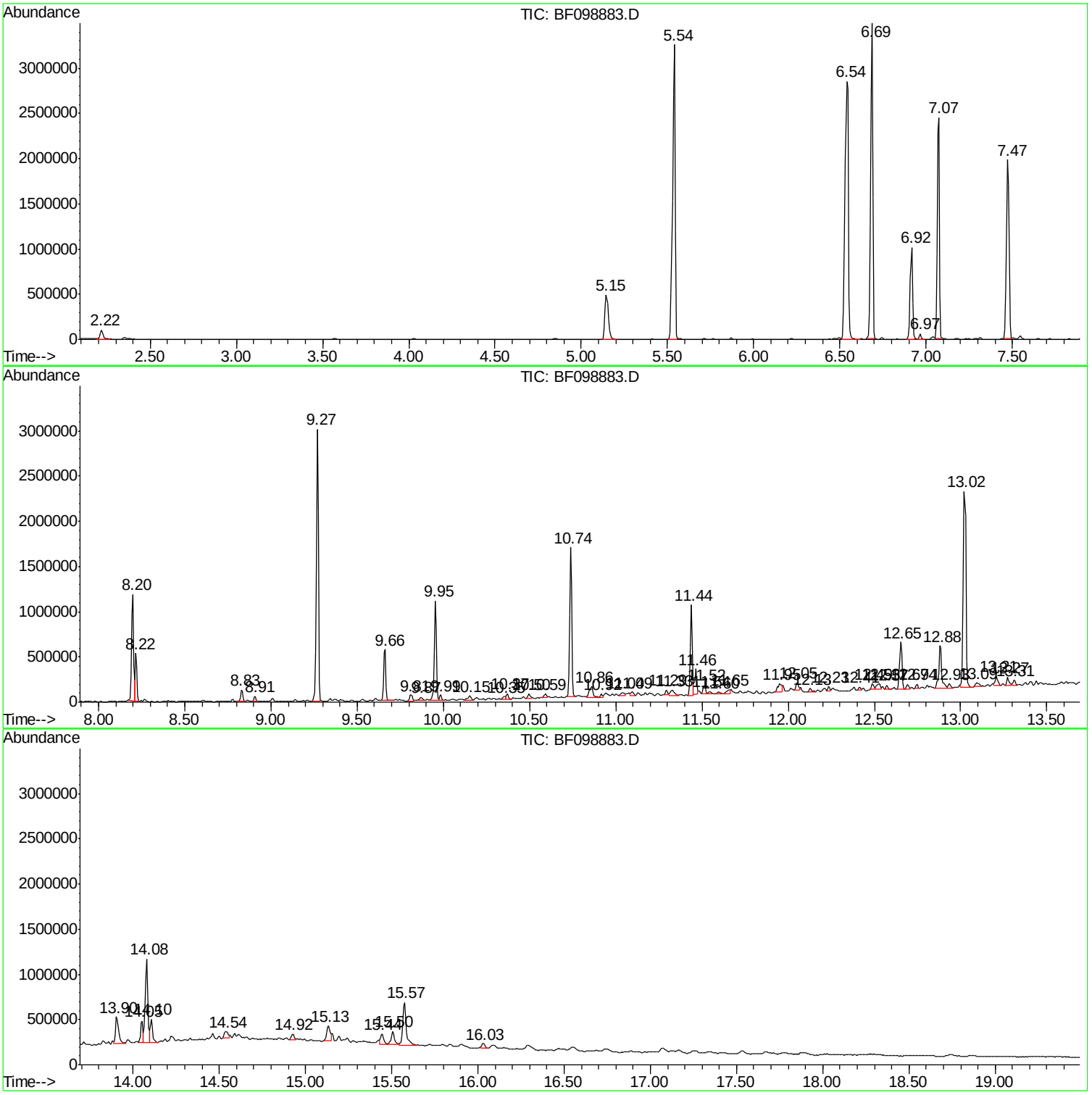
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ROLL-OFF1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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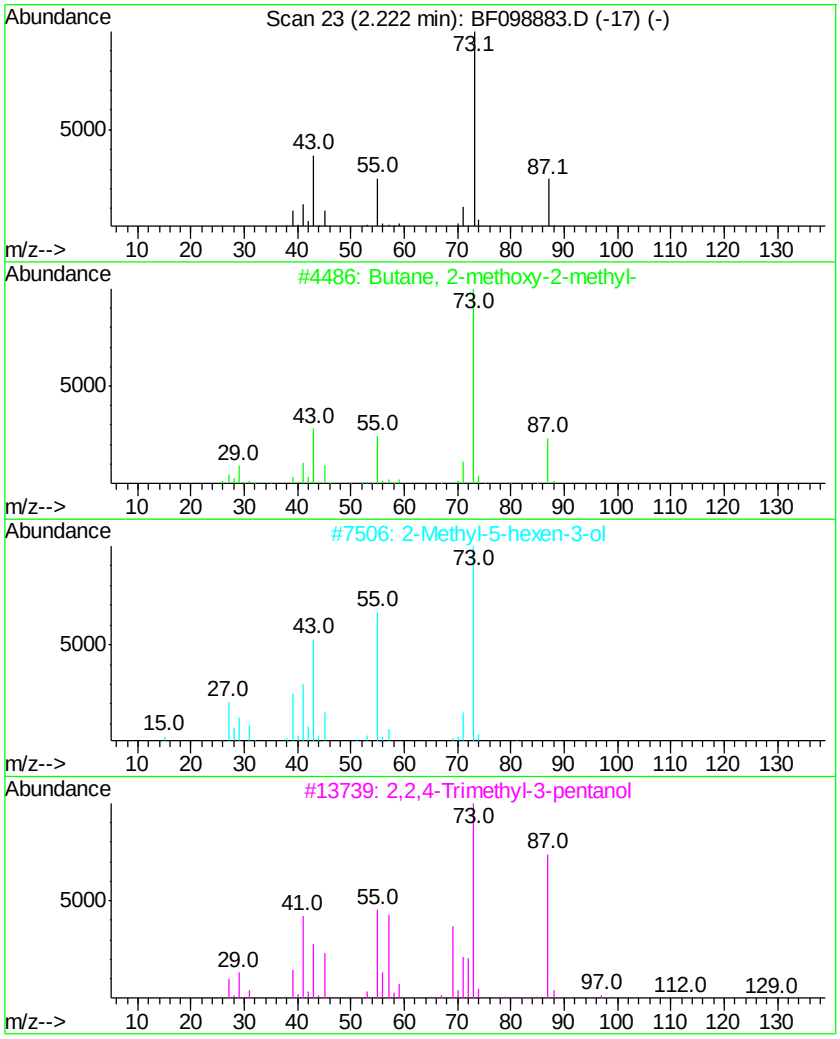
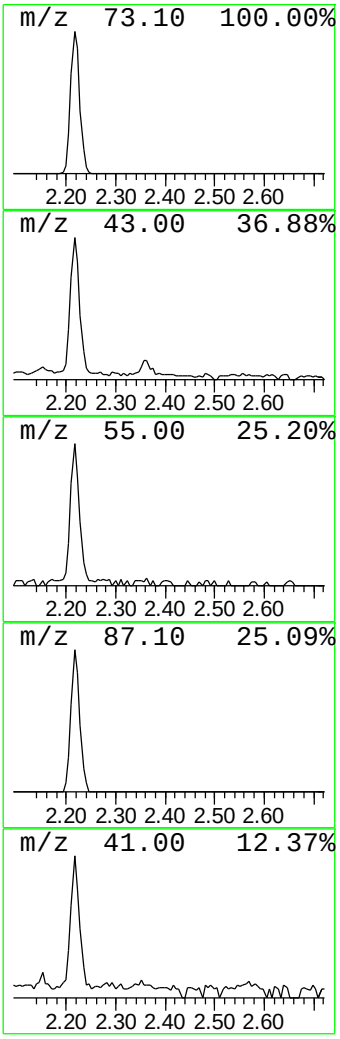
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	3.06 ng	126592	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	50
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
5	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	12





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Sample : I5249-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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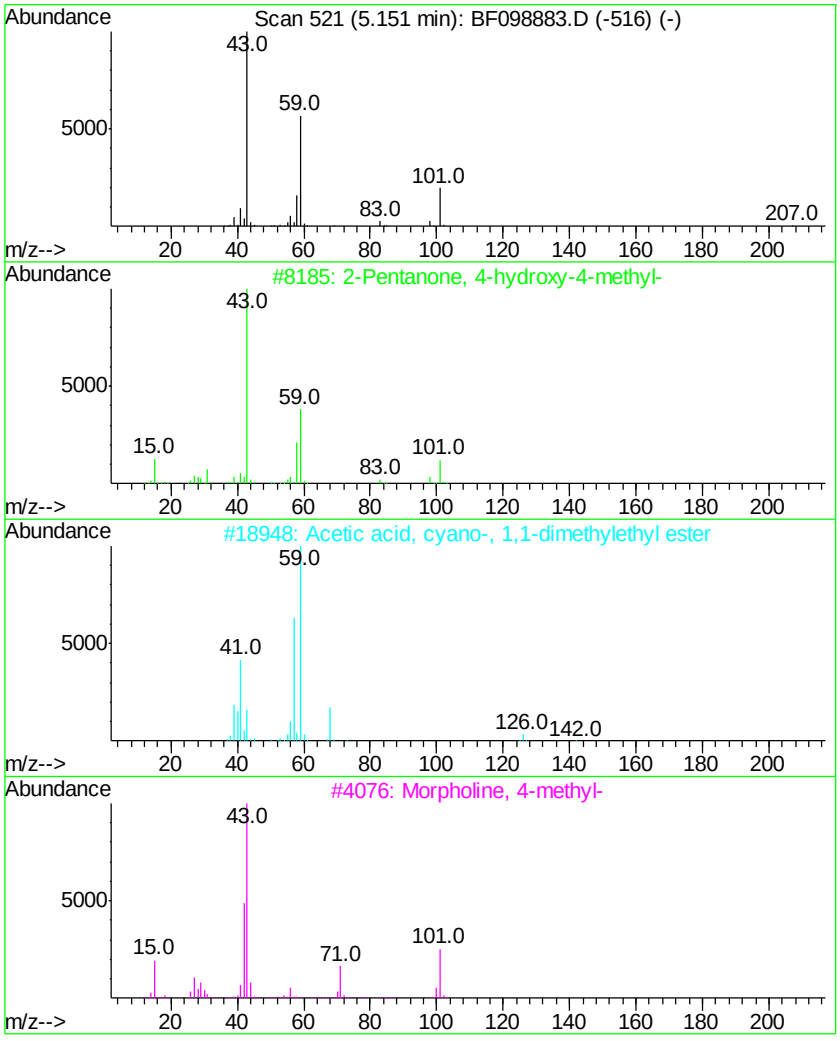
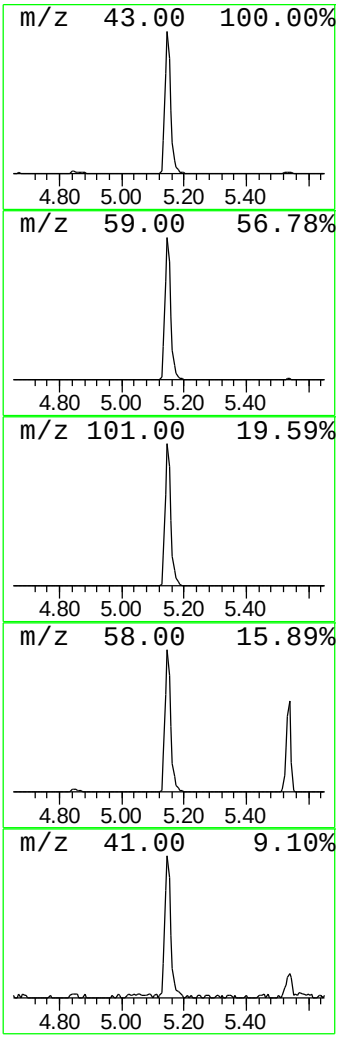
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	15.13 ng	626478	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9





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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Library : C:\DATABASE\NIST11.L
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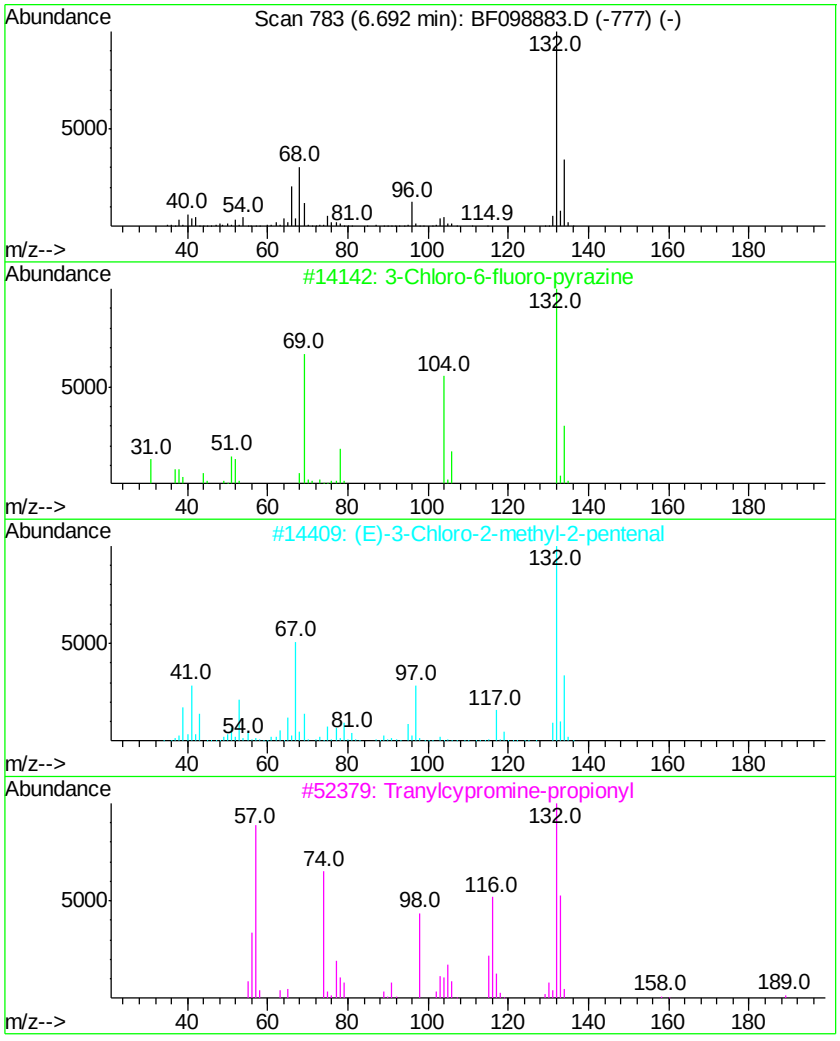
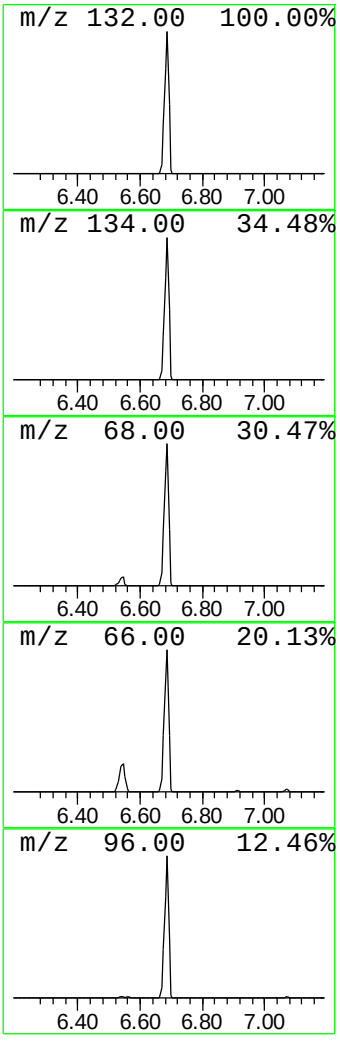
Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	80.16 ng	3318360	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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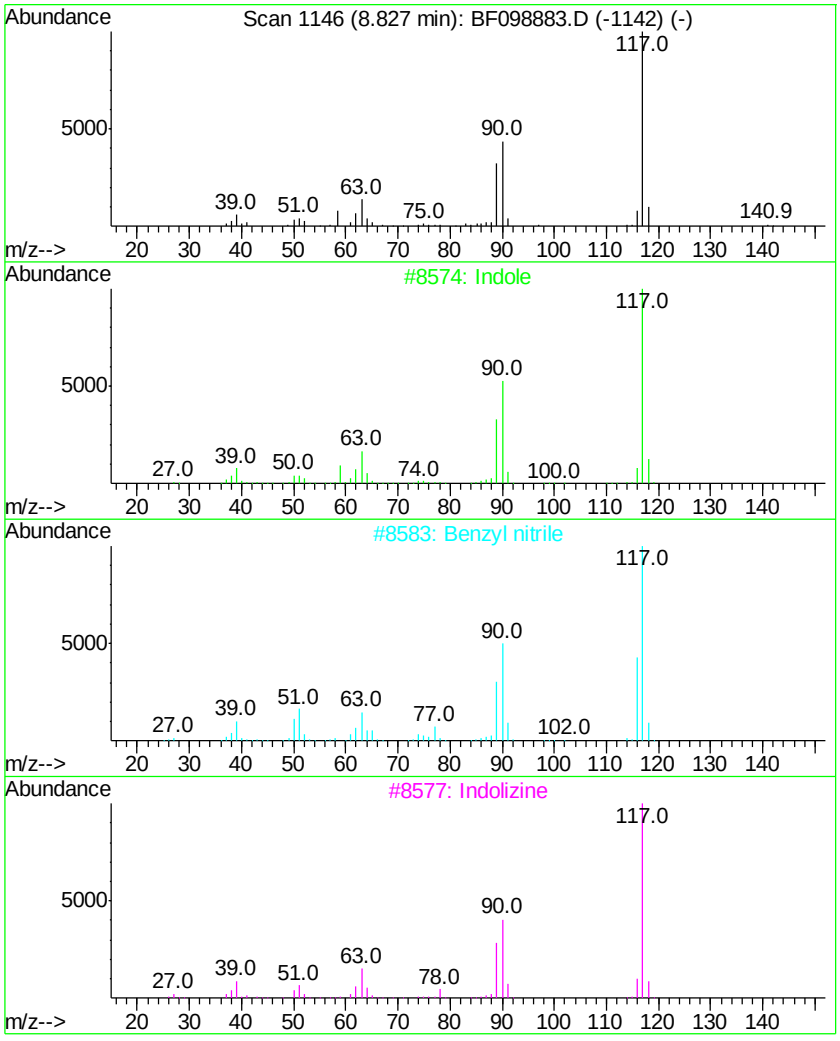
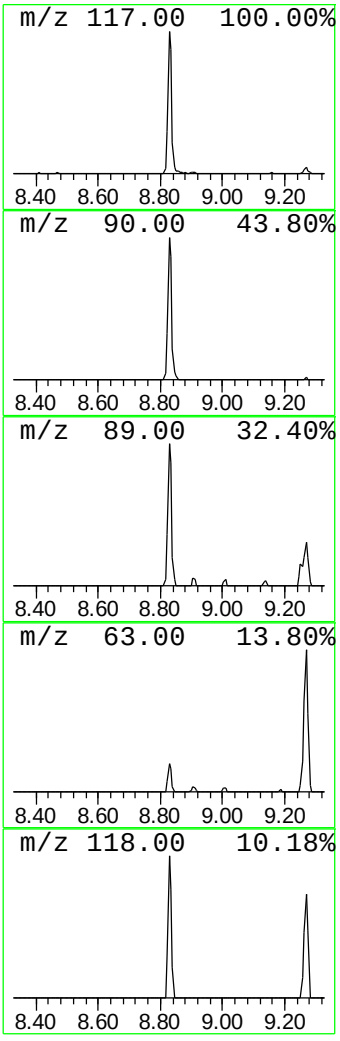
Peak Number 5 Indole Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.83	2.24 ng	121093	Naphthalene-d8	8.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indole	117	C8H7N	000120-72-9	97
2	Benzyl nitrile	117	C8H7N	000140-29-4	91
3	Indolizine	117	C8H7N	000274-40-8	91
4	Benzene, 1-isocyano-2-methyl-	117	C8H7N	010468-64-1	91
5	5H-1-Pyrindine	117	C8H7N	000270-91-7	91





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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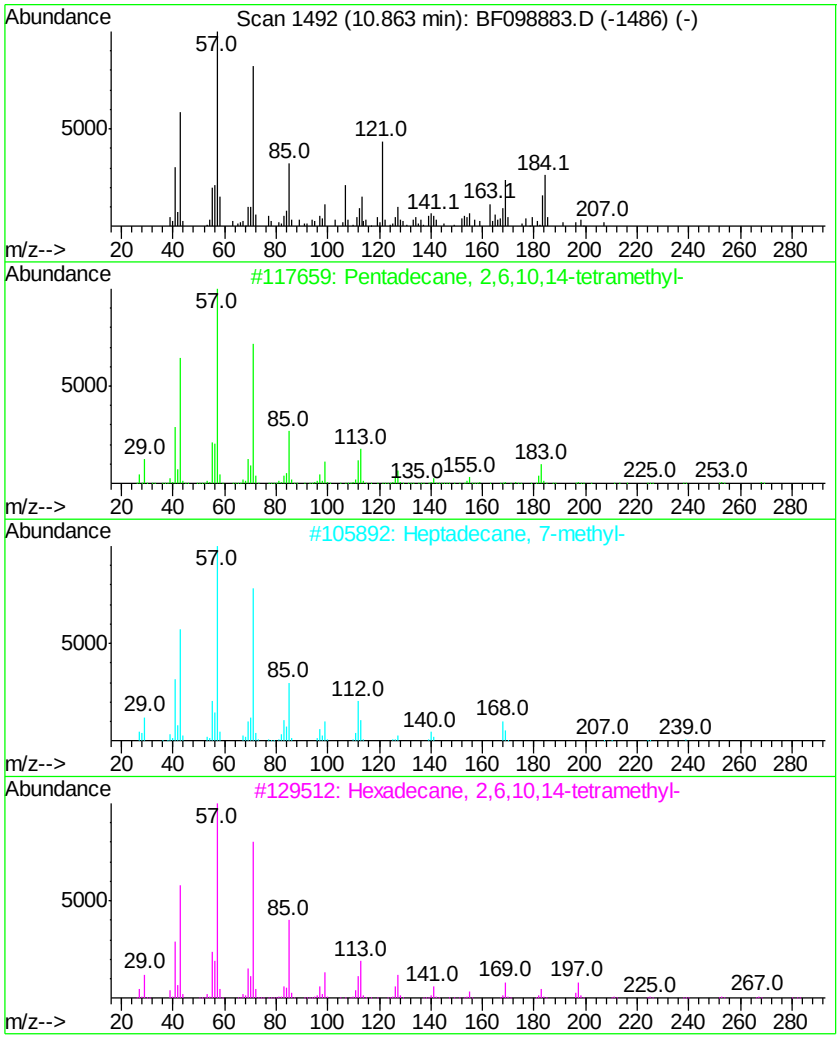
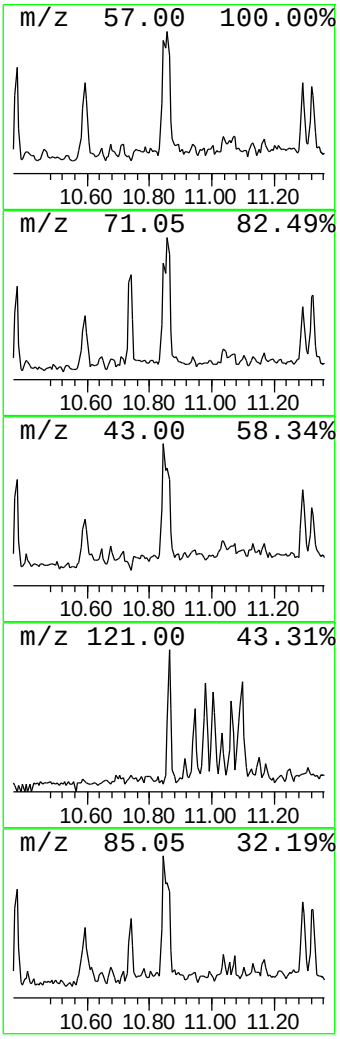
Peak Number 6 unknown10.86 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.86	4.63 ng	195444	Phenanthrene-d10	11.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	46
2	Heptadecane, 7-methyl-	254	C18H38	020959-33-5	46
3	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	45
4	3-Octen-2-ol, 2-methyl-, (Z)-	142	C9H18O	018521-07-8	43
5	Nonane, 2-methyl-5-propyl-	184	C13H28	031081-17-1	43





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TIC Library : C:\DATABASE\NIST11.L
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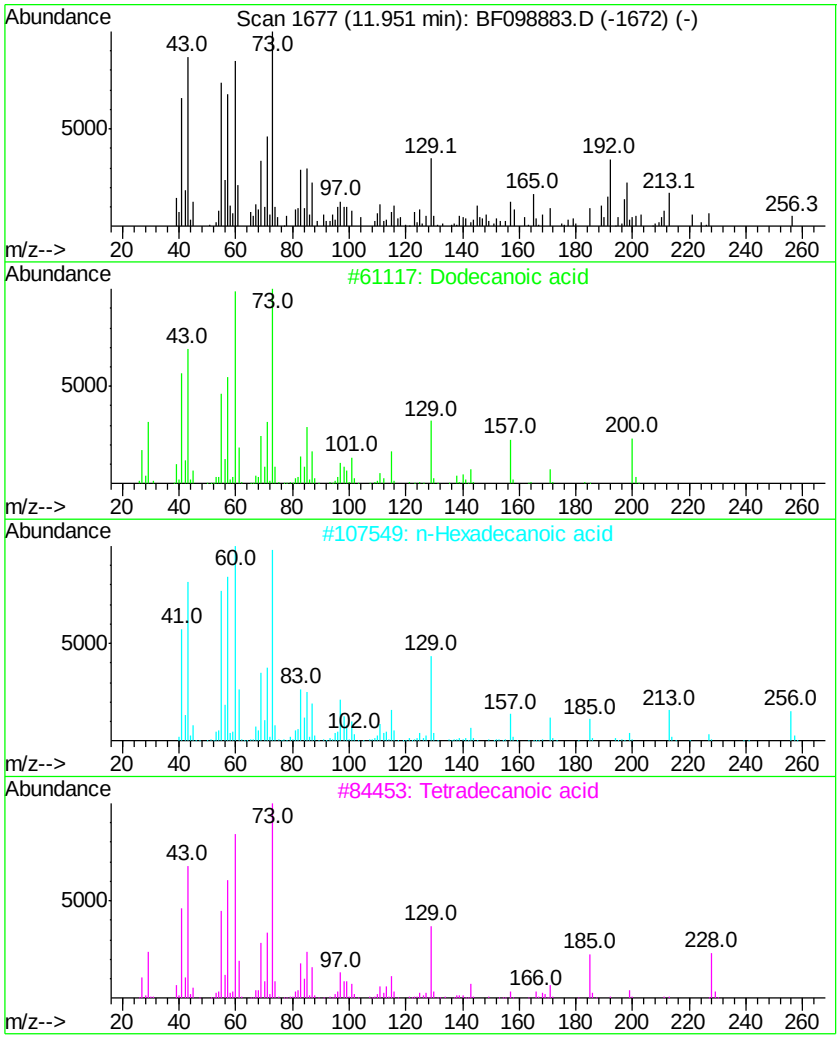
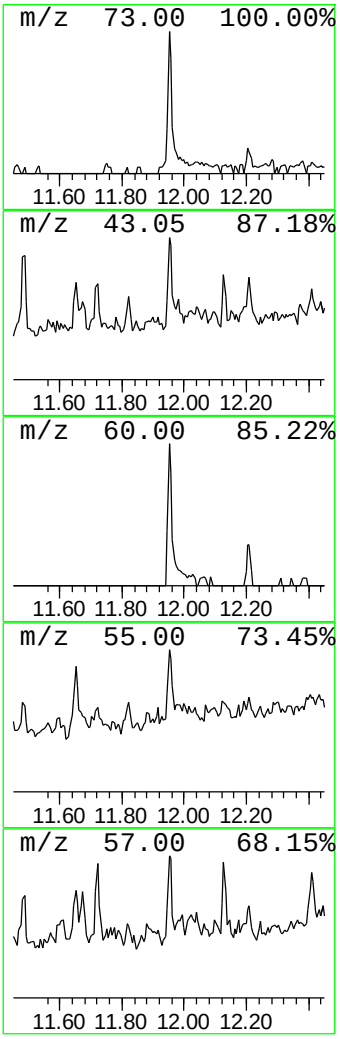
Peak Number 7 Dodecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	3.30 ng	139339	Phenanthrene-d10	11.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	76
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	58





Library Search Compound Report

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Data File : BF098883.D
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Operator : SJ/JU
Sample : I5249-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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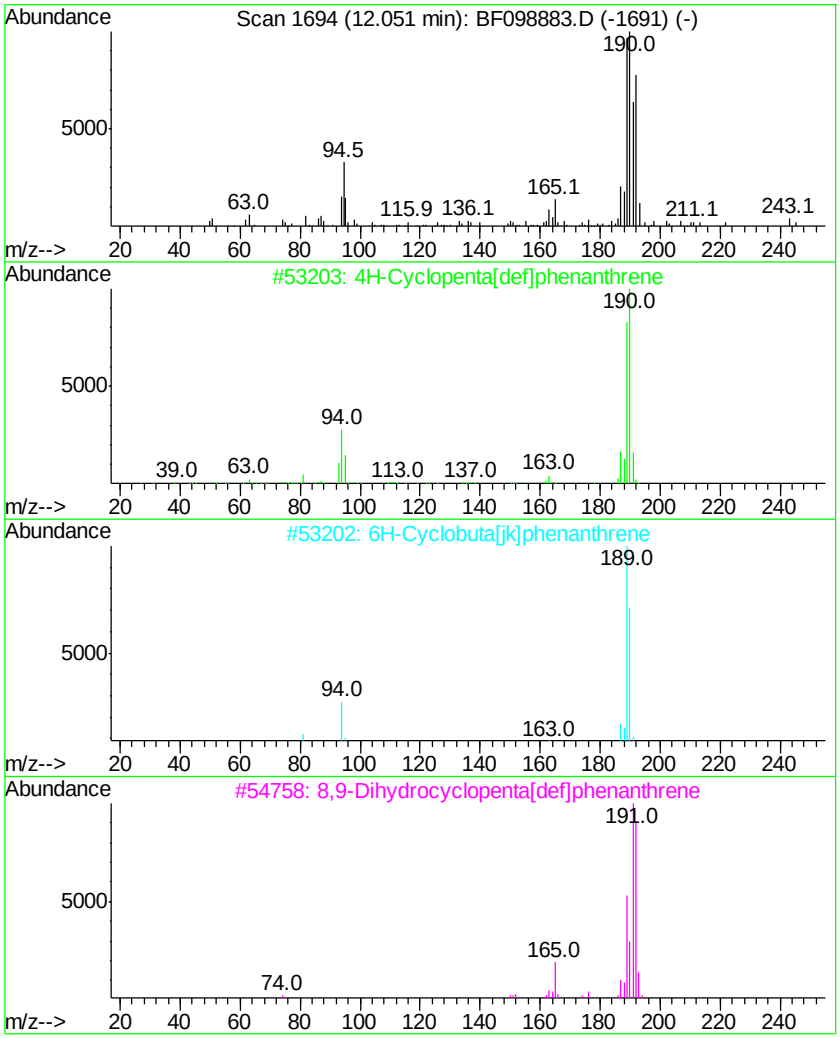
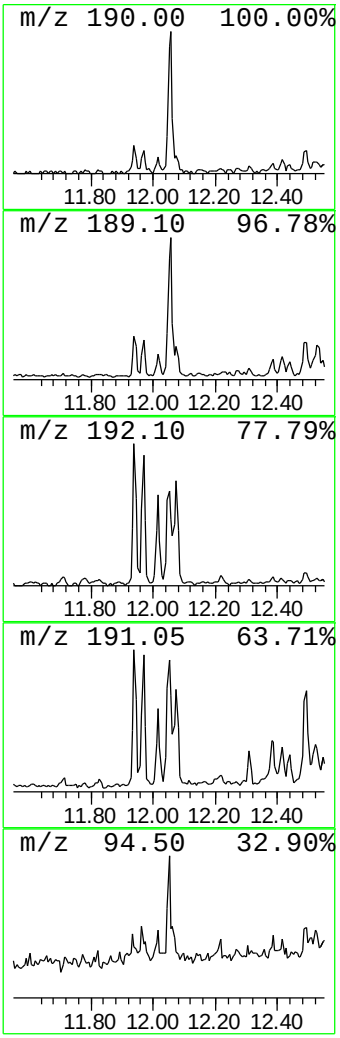
Peak Number 8 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	2.31 ng	97745	Phenanthrene-d10	11.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	92
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	49
3	8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	42
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	35
5	3-Bromo-2-furoic acid	190	C5H3BrO3	014903-90-3	35





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Acq On : 28 Sep 2017 00:48
Operator : SJ/JU
Sample : I5249-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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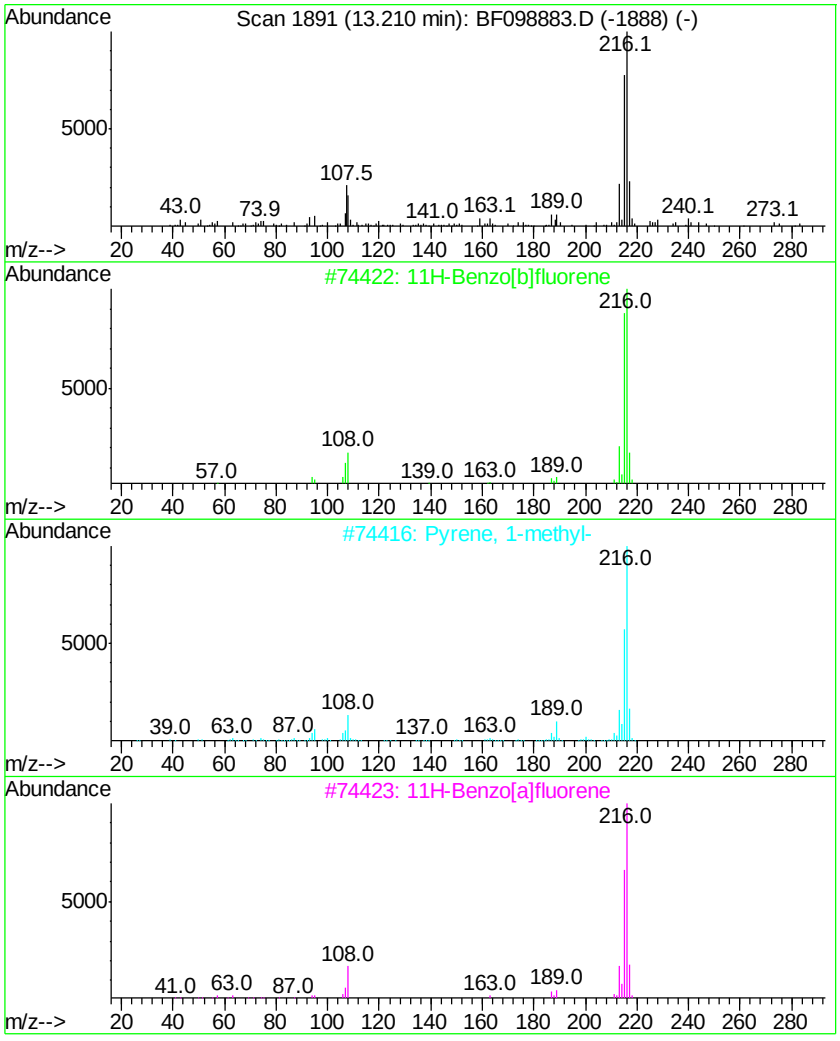
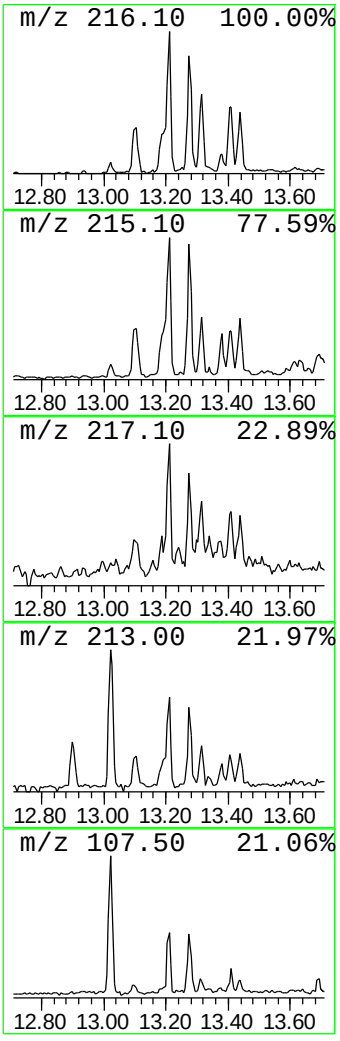
Peak Number 9 11H-Benzo[b]fluorene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.21	2.00 ng	106958	Chrysene-d12	14.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	86
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	81
4	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	72
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	70





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092717\
Data File : BF098883.D
Acq On : 28 Sep 2017 00:48
Operator : SJ/JU
Sample : I5249-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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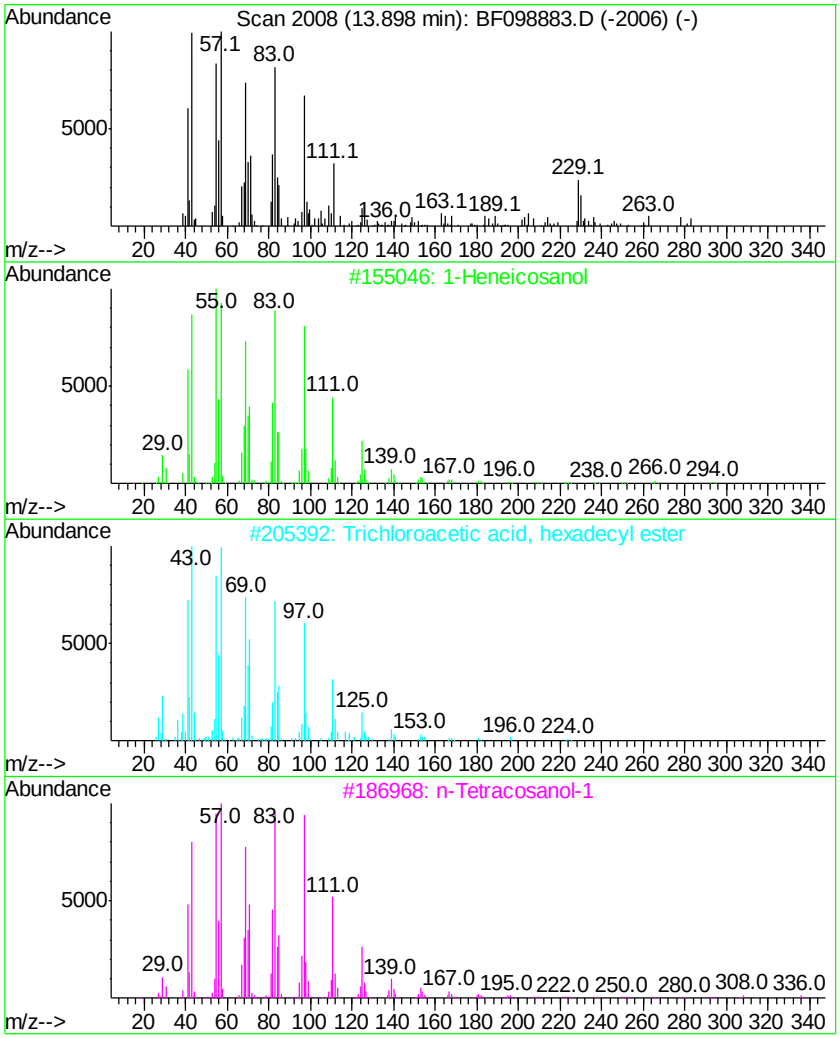
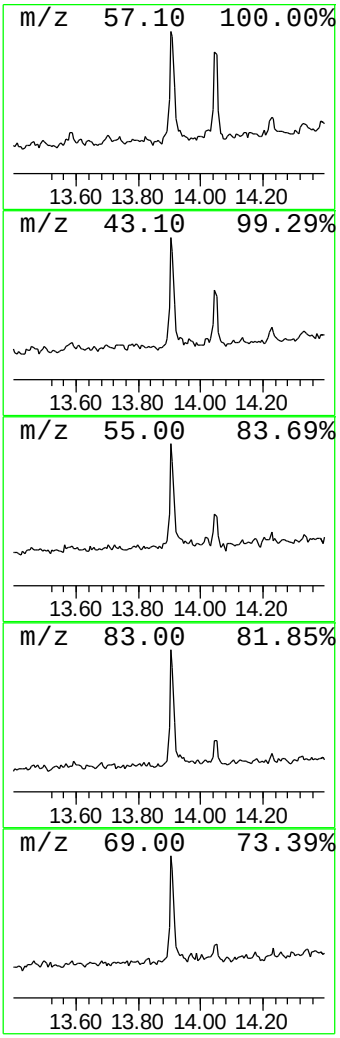
Peak Number 10 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	6.30 ng	336294	Chrysene-d12	14.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4	1-Docosene	308	C22H44	001599-67-3	90
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092717\
Data File : BF098883.D
Acq On : 28 Sep 2017 00:48
Operator : SJ/JU
Sample : I5249-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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
Butane, 2-methoxy...	2.22	3.1	ng	126592	1	6.92	827889	20.0
2-Pentanone, 4-hy...	5.15	15.1	ng	626478	1	6.92	827889	20.0
unknown6.69	6.69	80.2	ng	3318360	1	6.92	827889	20.0
Indole	8.83	2.2	ng	121093	2	8.20	1079870	20.0
unknown10.86	10.86	4.6	ng	195444	4	11.44	844622	20.0
Dodecanoic acid	11.95	3.3	ng	139339	4	11.44	844622	20.0
4H-Cyclopenta[def...	12.05	2.3	ng	97745	4	11.44	844622	20.0
11H-Benzo[b]fluorene	13.21	2.0	ng	106958	5	14.08	1068230	20.0
1-Heneicosanol	13.90	6.3	ng	336294	5	14.08	1068230	20.0