LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101917\
Data File : BF099666.D
Acq On : 19 Oct 2017 19:31
Operator : SJ/JU
Sample : I5896-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-19(0-10)COMP

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	5.039	499	502	521	rBV	244557	321116	18.89%	1.793%
2	5.451	568	572	587	rBV	1583167	1496656	88.06%	8.358%
3	6.463	740	744	762	rBV	1555634	1530796	90.07%	8.549%
4	6.592	762	766	770	rBV	1809872	1589896	93.55%	8.879%
5	6.822	801	805	813	rBB	595591	519111	30.54%	2.899%
6	6.975	827	831	835	rBV	1521448	1291664	76.00%	7.214%
7	7.386	897	901	904	rBV	1087834	954285	56.15%	5.329%
8	8.098	1019	1022	1026	rBV	819606	700166	41.20%	3.910%
9	9.174	1200	1205	1208	rBV	1969556	1699522	100.00%	9.491%
10	9.569	1269	1272	1278	rVB	46043	38744	2.28%	0.216%
11	9.851	1316	1320	1324	rBV	785138	696825	41.00%	3.892%
12	10.645	1451	1455	1464	rVB	845532	741951	43.66%	4.144%
13	11.339	1570	1573	1575	rBV	667388	543633	31.99%	3.036%
14	11.363	1575	1577	1582	rVV	262514	210097	12.36%	1.173%
15	11.416	1583	1586	1589	rVB	49951	43030	2.53%	0.240%
16	11.580	1610	1614	1618	rBV	18437	20299	1.19%	0.113%
17	11.839	1656	1658	1661	rBV	40466	48098	2.83%	0.269%
18	11.868	1661	1663	1669	rVB2	58023	55814	3.28%	0.312%
19	11.957	1674	1678	1680	rVV2	51665	63961	3.76%	0.357%
20	11.974	1680	1681	1686	rVB	30862	23931	1.41%	0.134%
21	12.133	1706	1708	1712	rBV	28484	25334	1.49%	0.141%
22	12.174	1712	1715	1719	rVB2	25140	22616	1.33%	0.126%
23	12.392	1746	1752	1754	rBV	36407	44343	2.61%	0.248%
24	12.486	1764	1768	1771	rBV3	26834	28926	1.70%	0.162%
25	12.557	1776	1780	1783	rBV	427073	365493	21.51%	2.041%
26	12.710	1800	1806	1807	rBV3	20013	27242	1.60%	0.152%
27	12.786	1816	1819	1824	rVB	413043	362590	21.33%	2.025%
28	12.833	1824	1827	1830	rVB2	21354	19022	1.12%	0.106%
29	12.921	1838	1842	1845	rVB	1159107	954179	56.14%	5.329%
30	13.004	1851	1856	1862	rBV3	28478	56757	3.34%	0.317%
31	13.092	1868	1871	1872	rBV2	24823	30141	1.77%	0.168%
32	13.110	1872	1874	1877	rVV	41904	45170	2.66%	0.252%
33	13.139	1877	1879	1881	rVB	29770	21892	1.29%	0.122%
34	13.215	1888	1892	1899	rBV2	41900	61009	3.59%	0.341%

LSC Area Percent Report

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Data File : BF099666.D
Acq On : 19 Oct 2017 19:31
Operator : SJ/JU
Sample : I5896-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-19(0-10)COMP

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

35	13.310	1905	1908	1910	rBV2	25651	20774	1.22%	0.116%
36	13.339	1910	1913	1920	rVV2	27826	34215	2.01%	0.191%
37	13.480	1934	1937	1940	rBV2	28211	29579	1.74%	0.165%
38	13.627	1959	1962	1964	rBV	45429	40199	2.37%	0.225%
39	13.733	1977	1980	1982	rBV	43633	43087	2.54%	0.241%
40	13.757	1982	1984	1987	rVV	42355	35812	2.11%	0.200%
41	13.786	1987	1989	1990	rVV	35076	33204	1.95%	0.185%
42	13.804	1990	1992	1995	rVV2	122994	126362	7.44%	0.706%
43	13.839	1995	1998	2004	rVB	67023	70858	4.17%	0.396%
44	13.945	2013	2016	2018	rBV	36912	31532	1.86%	0.176%
45	13.980	2018	2022	2025	rVV2	562999	718446	42.27%	4.012%
46	14.009	2025	2027	2031	rVB	230812	188949	11.12%	1.055%
47	14.092	2038	2041	2043	rBV	26962	23635	1.39%	0.132%
48	14.121	2044	2046	2048	rBV	27125	19875	1.17%	0.111%
49	14.333	2080	2082	2084	rBV	25684	21604	1.27%	0.121%
50	14.368	2086	2088	2091	rVB	42989	33454	1.97%	0.187%
51	14.427	2095	2098	2099	rBV2	42028	37103	2.18%	0.207%
52	14.868	2170	2173	2176	rBV2	45638	49464	2.91%	0.276%
53	15.021	2195	2199	2202	rBV	225702	307220	18.08%	1.716%
54	15.133	2215	2218	2221	rBV	44350	49386	2.91%	0.276%
55	15.321	2247	2250	2255	rVB	132291	147961	8.71%	0.826%
56	15.386	2257	2261	2265	rBV	201912	242291	14.26%	1.353%
57	15.445	2267	2271	2275	rVV	371110	426505	25.10%	2.382%
58	15.851	2337	2340	2343	rVB2	40421	49542	2.92%	0.277%
59	16.915	2516	2521	2529	rVB	126959	239150	14.07%	1.336%
60	17.362	2592	2597	2603	rVB	73110	150825	8.87%	0.842%
61	17.597	2633	2637	2645	rVB5	32019	80472	4.73%	0.449%

Sum of corrected areas: 17905813

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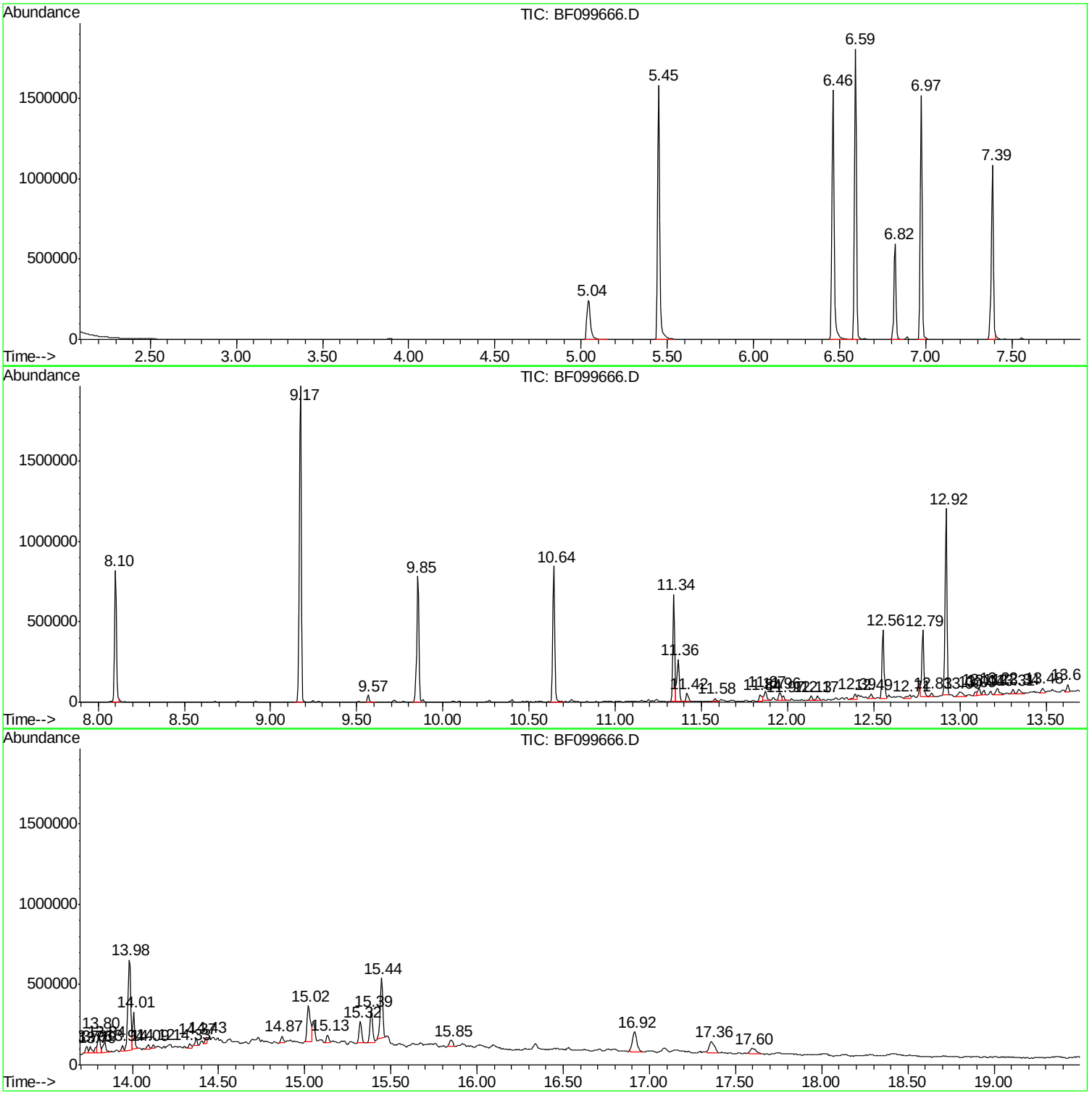
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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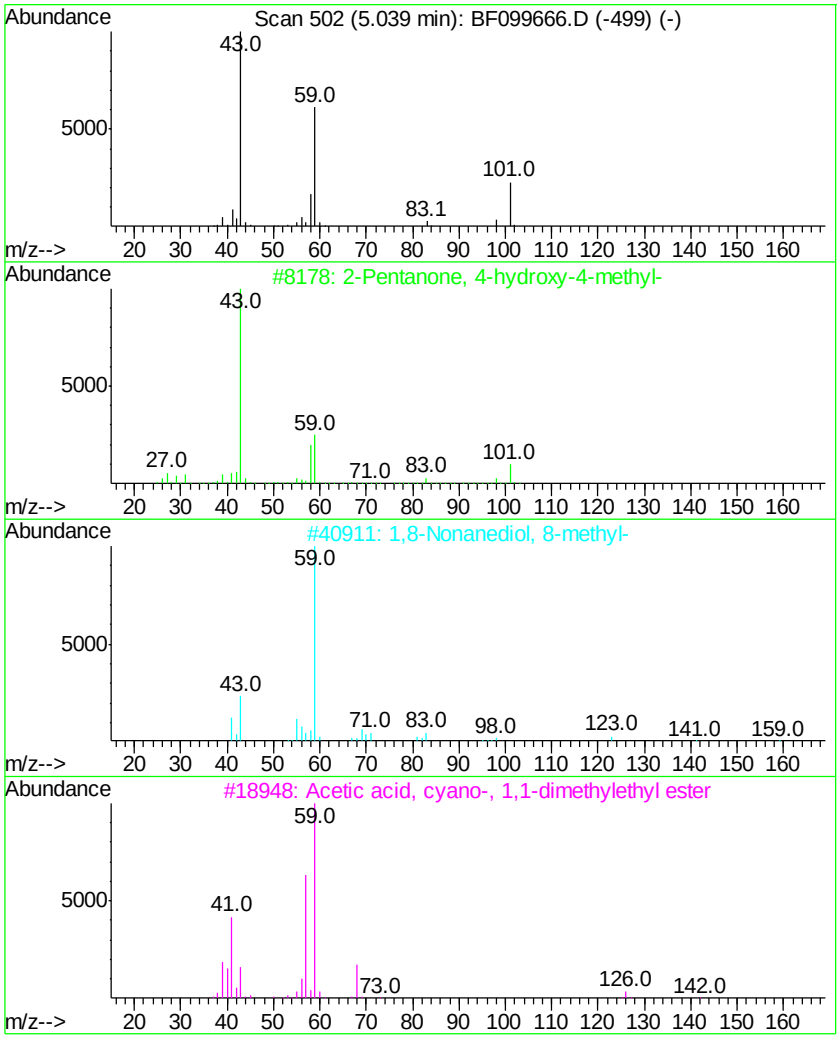
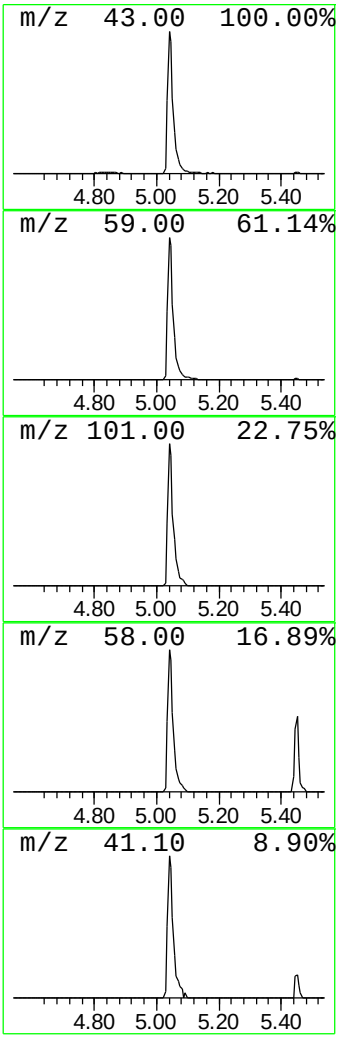
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	12.37 ng	321116	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	17
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101917\
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Operator : SJ/JU
Sample : I5896-01
Misc :
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Instrument : BNA_F
ClientSampleId : B-19(0-10)COMP

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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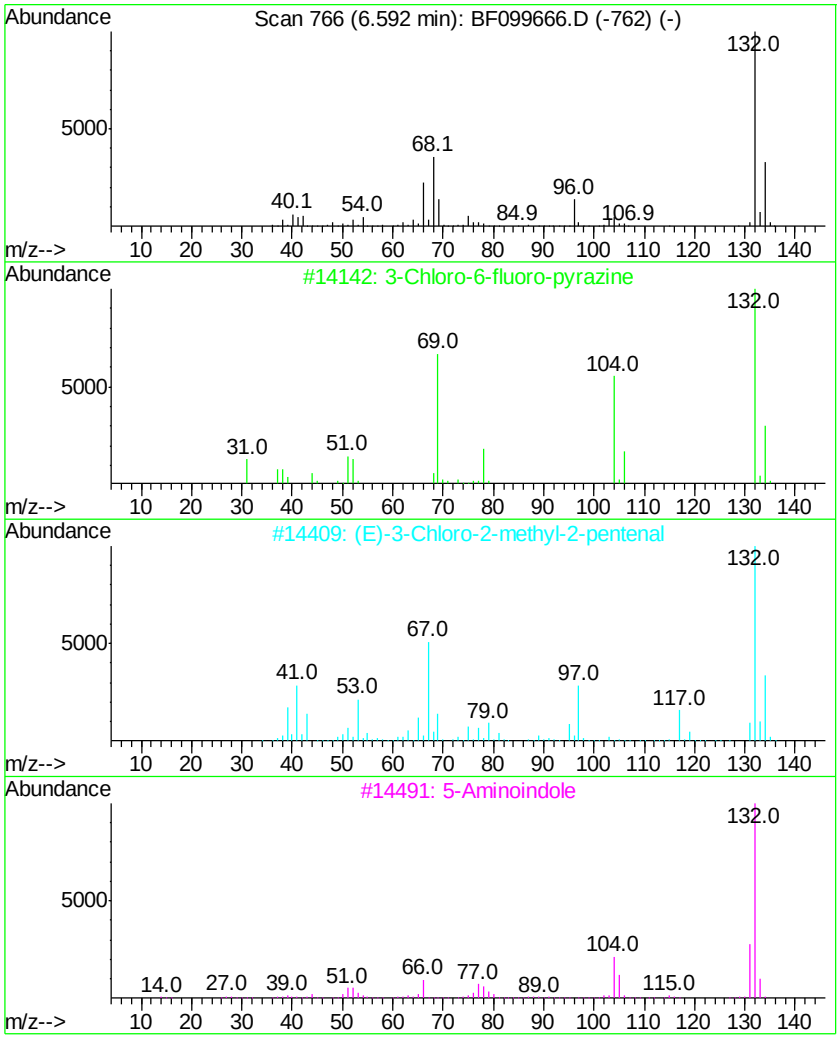
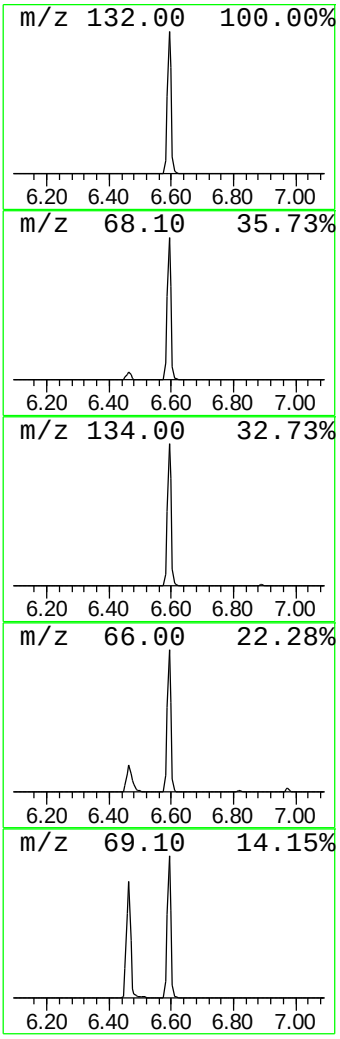
Peak Number 2 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	61.25 ng	1589900	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Instrument : BNA_F
ClientSampleId : B-19(0-10)COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Library : C:\DATABASE\NIST11.L
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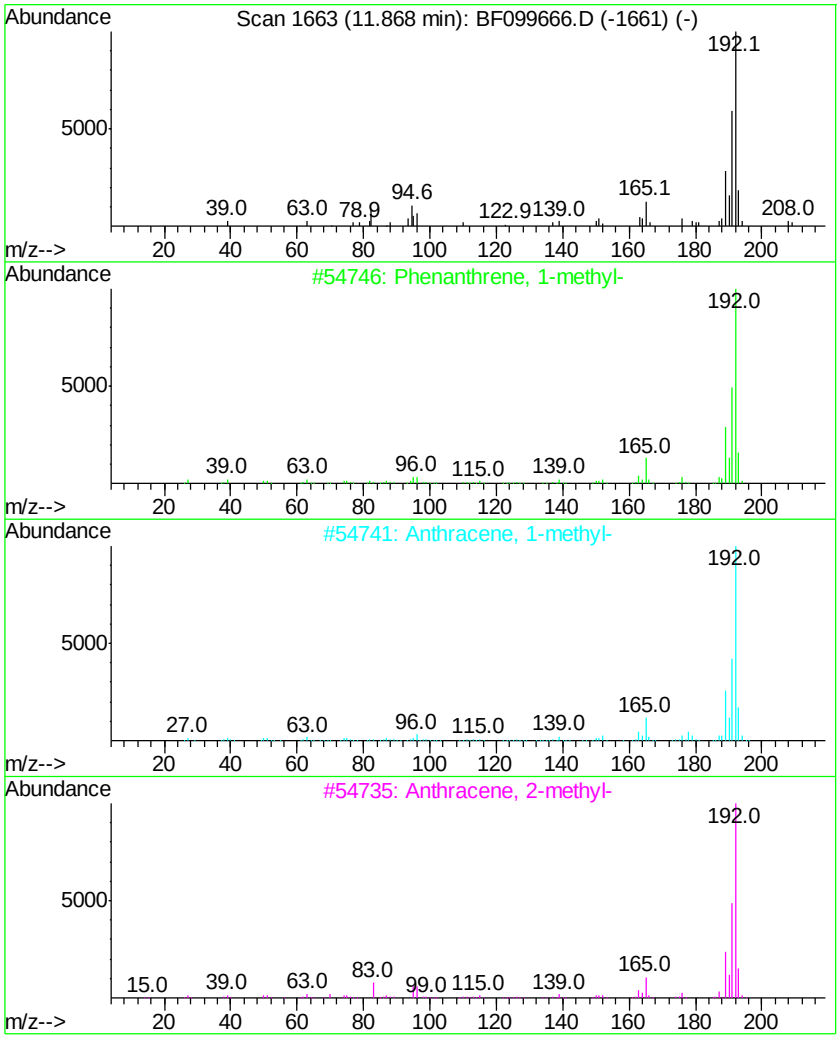
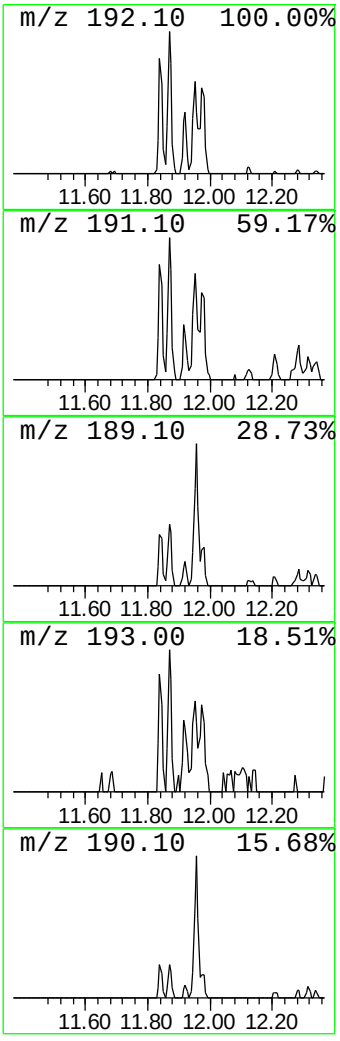
Peak Number 4 Phenanthrene, 1-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	2.05 ng	55814	Phenanthrene-d10	11.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	94
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	90





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Instrument : BNA_F
ClientSampleId : B-19(0-10)COMP

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

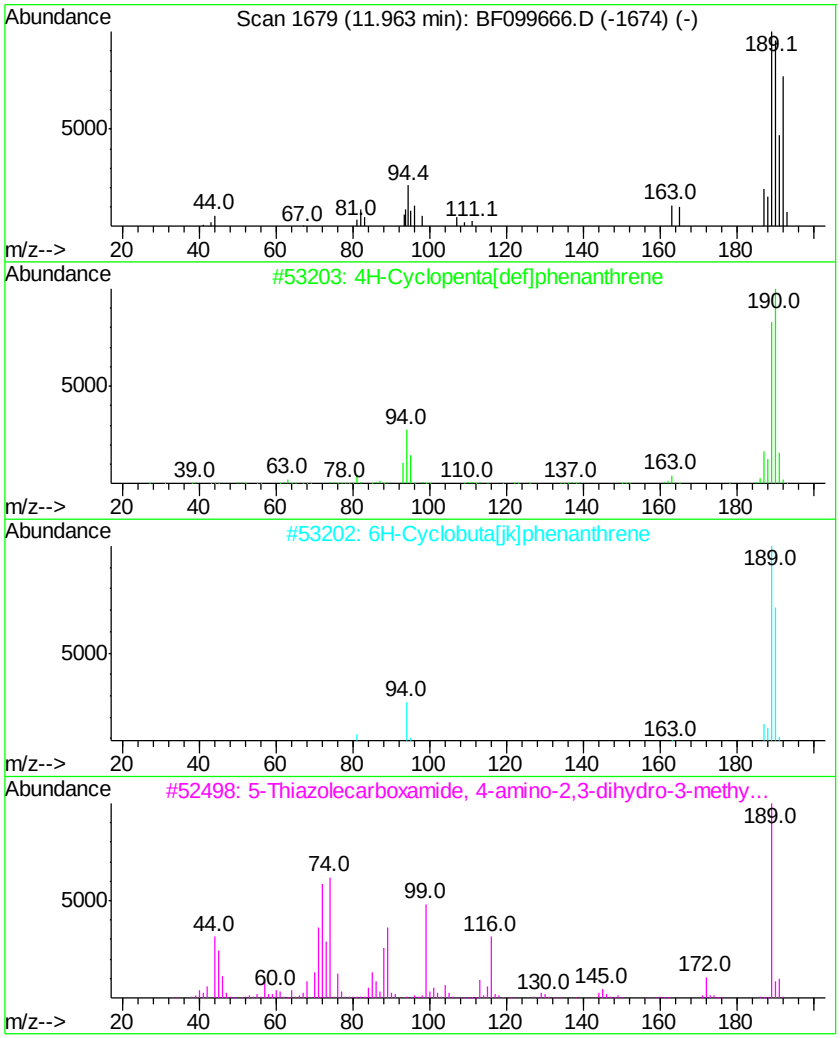
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

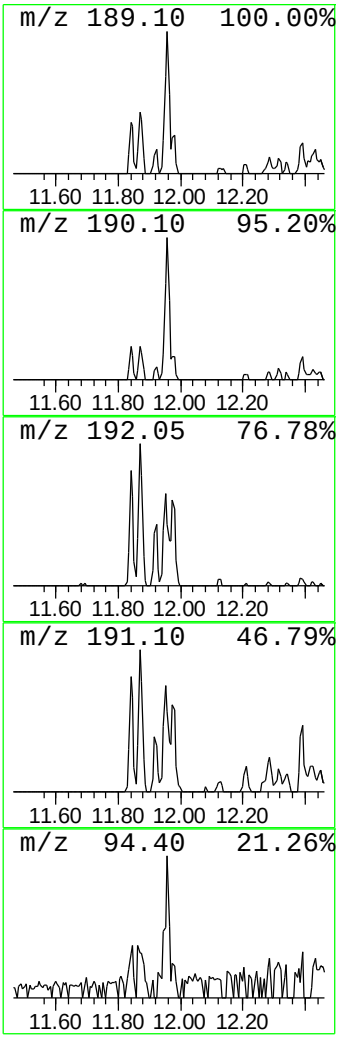
****

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	2.35 ng	63961	Phenanthrene-d10	11.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	76
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	53
3	5-Thiazolecarboxamide, 4-amino-2...	189	C5H7N3OS2	1000338-08-9	22
4	Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	18
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	14





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Instrument : BNA_F
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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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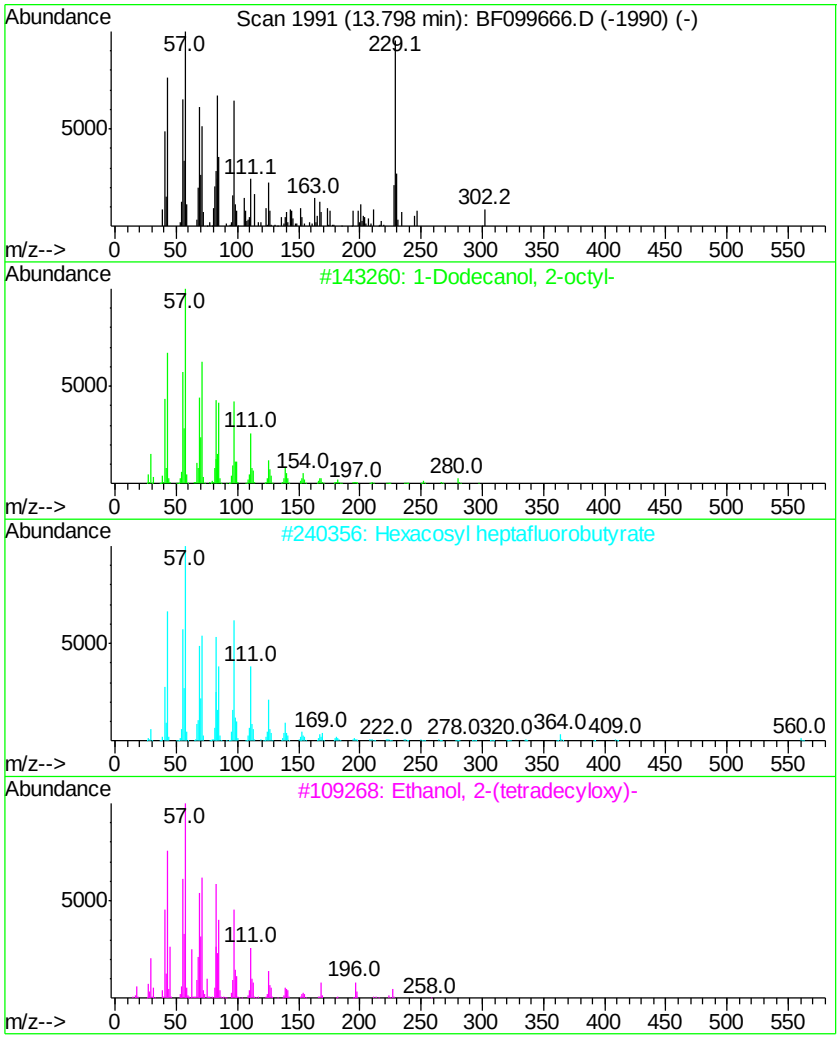
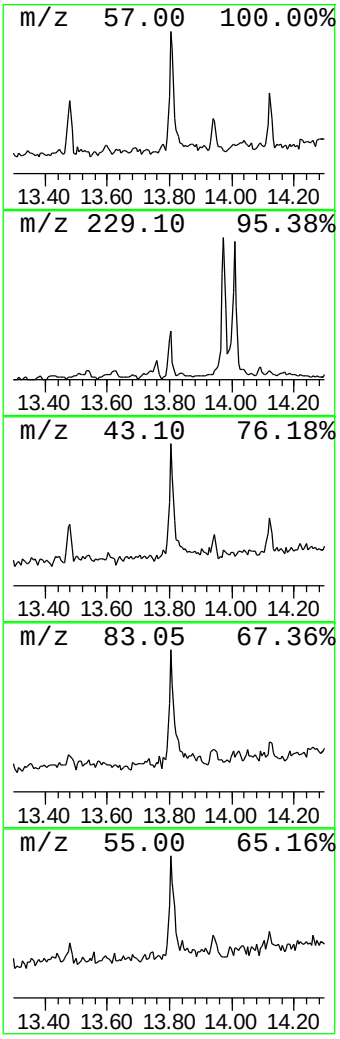
Peak Number 6 1-Dodecanol, 2-octyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	3.52 ng	126362	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	68
2	Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	68
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	64
4	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	58
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	55





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Instrument : BNA_F
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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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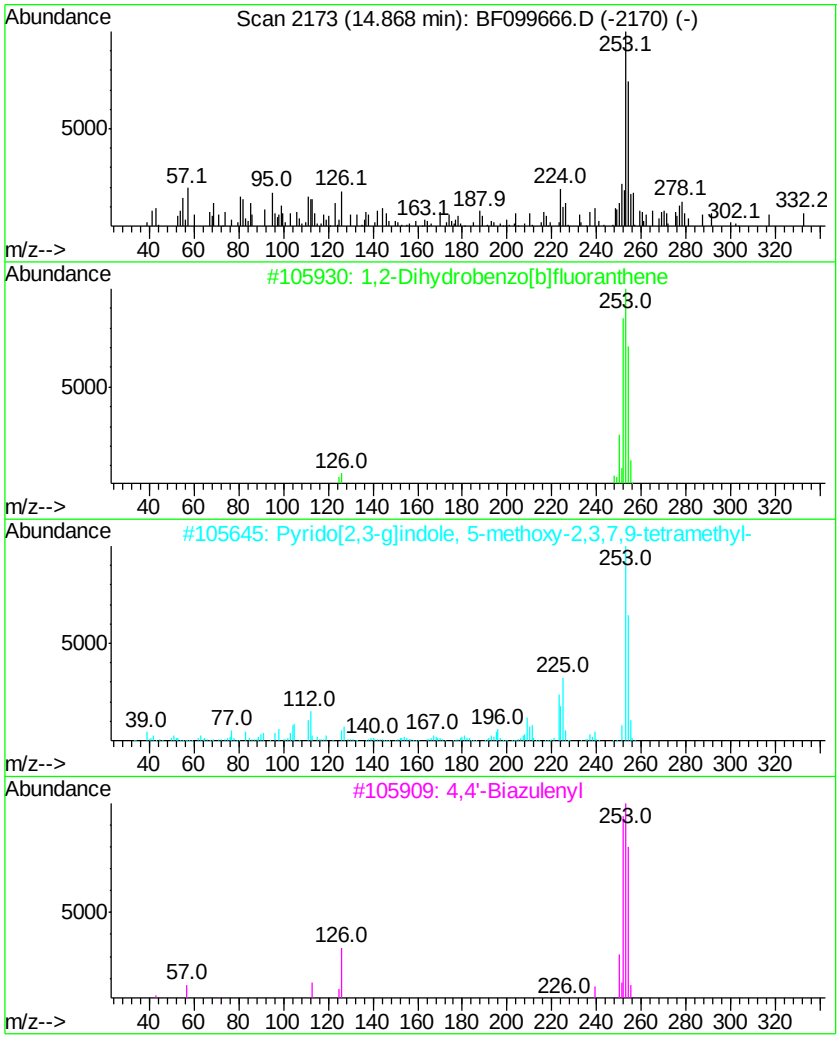
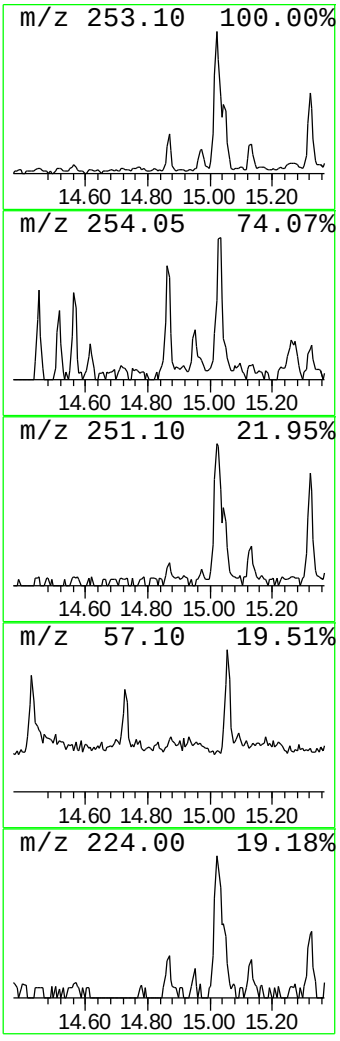
Peak Number 7 1,2-Dihydrobenzo[b]fluorant... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	2.32 ng	49464	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Dihydrobenzo[b]fluoranthene	254	C20H14	100516-13-0	53
2	Pyrido[2,3-g]indole, 5-methoxy-2...	254	C16H18N2O	201991-45-9	53
3	4,4'-Biazulenyl	254	C20H14	094053-54-0	52
4	4,6'-Biazulenyl	254	C20H14	094154-49-1	52
5	3H-Pyrrolo[3,2-f]quinoline, 5-me...	254	C16H18N2O	1000350-44-1	50





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Instrument : BNA_F
ClientSampleId : B-19(0-10)COMP

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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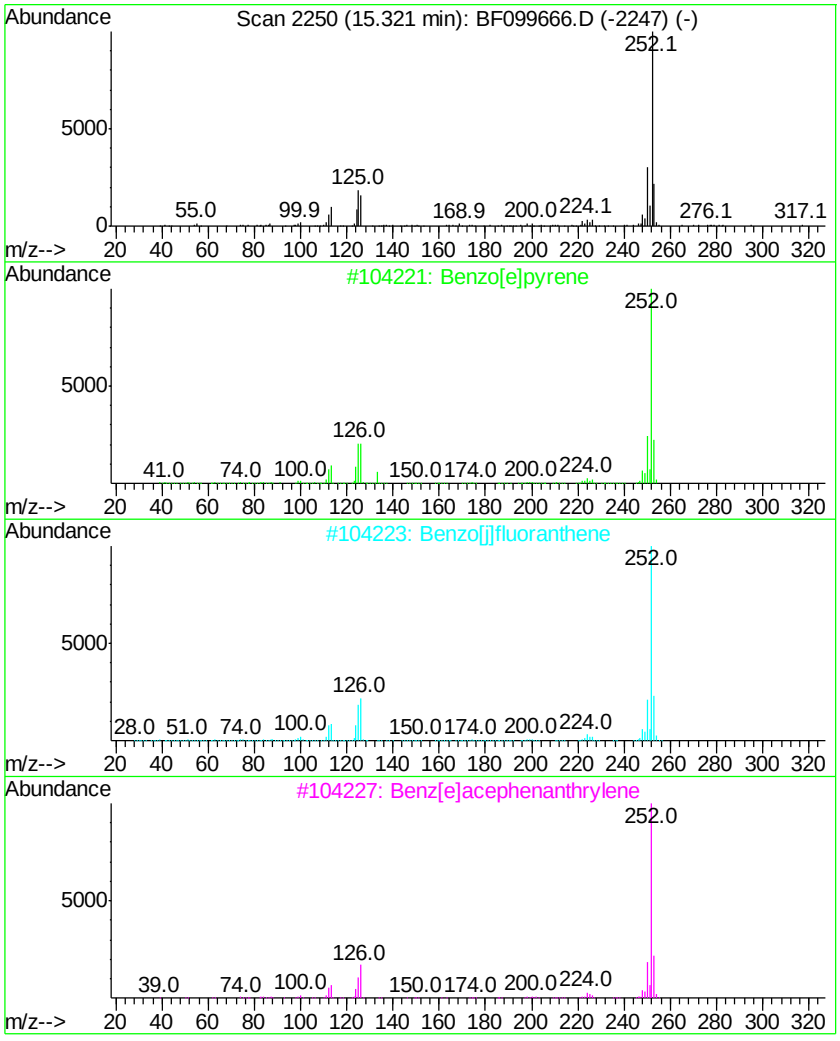
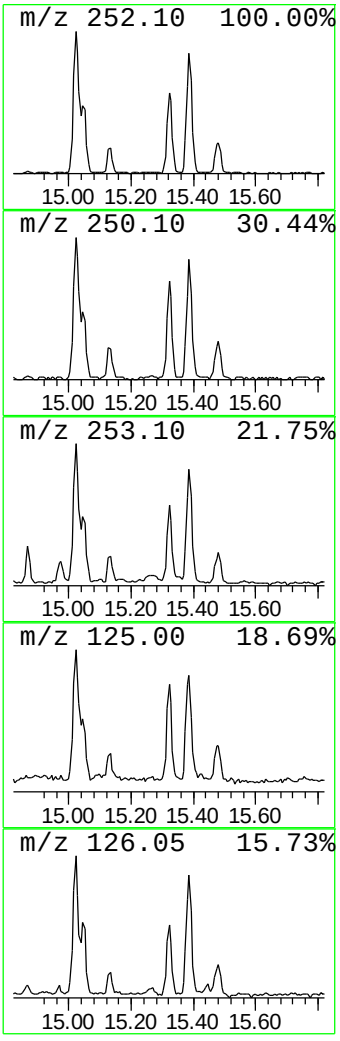
Peak Number 9 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.32	6.94 ng	147961	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[j]fluoranthene	252	C20H12	000205-82-3	98
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	97
4	Perylene	252	C20H12	000198-55-0	97
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93





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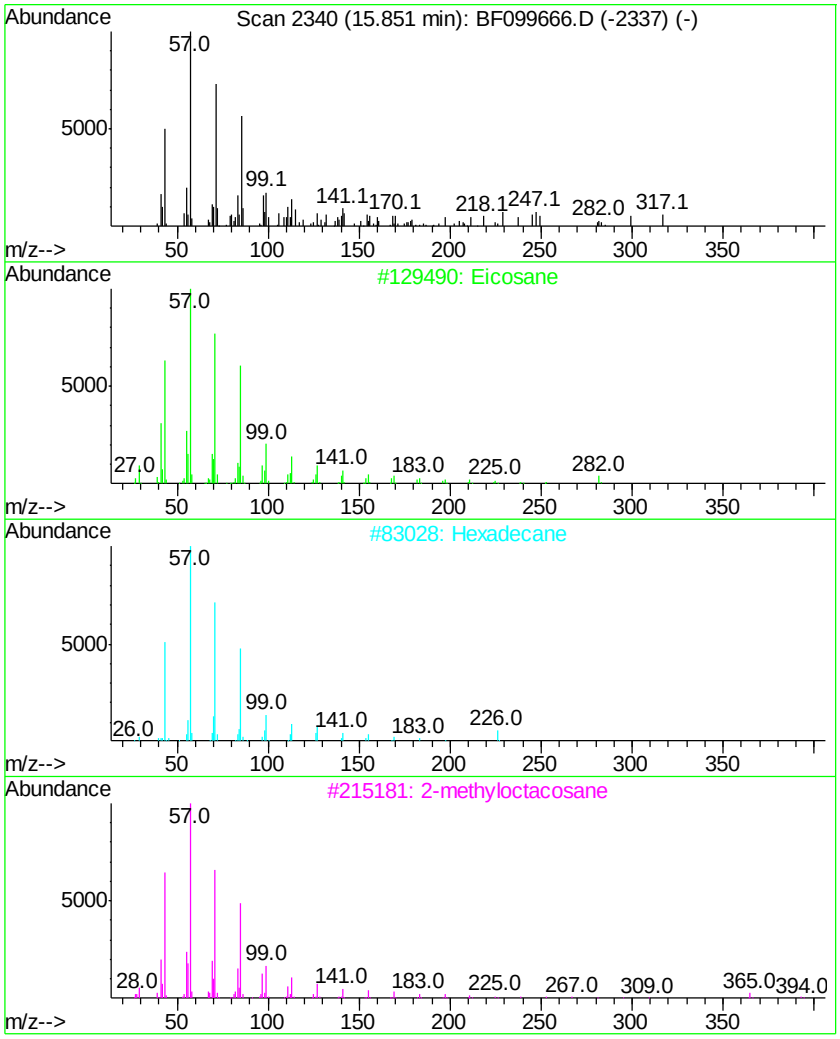
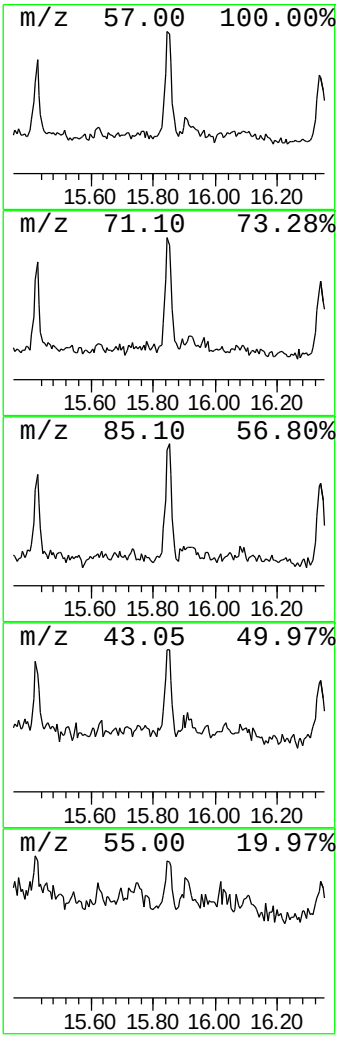
Peak Number 10 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.85	2.32 ng	49542	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	89
2	Hexadecane	226	C16H34	000544-76-3	76
3	2-methyloctacosane	408	C29H60	1000376-72-8	64
4	Heneicosane	296	C21H44	000629-94-7	64
5	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101917\
Data File : BF099666.D
Acq On : 19 Oct 2017 19:31
Operator : SJ/JU
Sample : I5896-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-19(0-10)COMP

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
2-Pentanone, 4-hy...	5.04	12.4	ng	321116	1	6.82	519111	20.0
unknown6.59	6.59	61.3	ng	1589900	1	6.82	519111	20.0
Phenanthrene, 1-m...	11.87	2.0	ng	55814	4	11.34	543633	20.0
4H-Cyclopenta[def...	11.96	2.4	ng	63961	4	11.34	543633	20.0
1-Dodecanol, 2-oc...	13.80	3.5	ng	126362	5	13.99	718446	20.0
1,2-Dihydrobenzo[...	14.87	2.3	ng	49464	6	15.44	426505	20.0
Benzo[e]pyrene	15.32	6.9	ng	147961	6	15.44	426505	20.0
Eicosane	15.85	2.3	ng	49542	6	15.44	426505	20.0