LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022221\
Data File : BF123268.D
Acq On : 22 Feb 2021 20:20
Operator : JU/CG
Sample : M1452-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123268.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	12	rVB	457771	542828	11.95%	1.539%
2	5.481	572	577	580	rBV	3432542	3157308	69.52%	8.952%
3	6.493	743	749	761	rBV2	3161772	3613843	79.57%	10.246%
4	6.857	807	811	814	rBV	885368	741476	16.33%	2.102%
5	7.416	901	906	909	rBV	2144579	2094074	46.11%	5.937%
6	8.139	1025	1029	1032	rBV	1525773	1233204	27.15%	3.496%
7	9.216	1207	1212	1216	rBV	4226282	4053690	89.26%	11.493%
8	9.610	1276	1279	1283	rBV	131865	100772	2.22%	0.286%
9	9.898	1324	1328	1331	rBV	1679326	1357744	29.90%	3.849%
10	10.692	1458	1463	1473	rBV	2663862	2739706	60.33%	7.768%
11	11.239	1553	1556	1561	rBV4	44298	70312	1.55%	0.199%
12	11.386	1577	1581	1584	rBV	1784523	1649438	36.32%	4.676%
13	11.410	1584	1585	1589	rVV	459399	299854	6.60%	0.850%
14	11.463	1589	1594	1597	rVB	95748	121700	2.68%	0.345%
15	11.616	1615	1620	1623	rBV2	45605	60135	1.32%	0.170%
16	11.745	1639	1642	1646	rVB	97687	76443	1.68%	0.217%
17	11.892	1664	1667	1669	rBV	64552	58874	1.30%	0.167%
18	11.916	1669	1671	1678	rVV2	284650	354874	7.81%	1.006%
19	12.004	1683	1686	1688	rVV2	102324	125319	2.76%	0.355%
20	12.027	1688	1690	1694	rVB	56726	51450	1.13%	0.146%
21	12.210	1719	1721	1725	rVB	69907	60151	1.32%	0.171%
22	12.369	1745	1748	1751	rBV	120367	99567	2.19%	0.282%
23	12.527	1772	1775	1780	rVB2	54303	58467	1.29%	0.166%
24	12.604	1784	1788	1793	rBV	835865	710661	15.65%	2.015%
25	12.710	1802	1806	1812	rBV4	90794	165146	3.64%	0.468%
26	12.833	1819	1827	1830	rBV	715291	730482	16.08%	2.071%
27	12.880	1833	1835	1841	rVB3	58316	70147	1.54%	0.199%
28	12.980	1848	1852	1856	rBV	4549113	4541496	100.00%	12.876%
29	13.051	1860	1864	1868	rVB4	47304	69508	1.53%	0.197%
30	13.139	1876	1879	1881	rBV4	43745	49327	1.09%	0.140%
31	13.163	1881	1883	1887	rVB	94047	86364	1.90%	0.245%
32	13.210	1887	1891	1893	rBV3	43655	50453	1.11%	0.143%
33	13.269	1897	1901	1904	rBV2	83069	87372	1.92%	0.248%
34	13.392	1919	1922	1926	rBV2	47487	45751	1.01%	0.130%
35	13.457	1929	1933	1940	rVB5	41496	65810	1.45%	0.187%
36	13.674	1967	1970	1976	rVB	78274	81303	1.79%	0.231%

LSC Area Percent Report

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Sample : M1452-05
Misc :
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Instrument : BNA_F
ClientSampleId : TP-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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.780	1983	1988	1991	rBV2	59255	88759	1.95%	0.252%
38	13.816	1991	1994	1996	rVV	57443	50938	1.12%	0.144%
39	13.886	2002	2006	2007	rBV2	103339	113472	2.50%	0.322%
40	13.916	2007	2011	2024	rVV5	139611	476840	10.50%	1.352%
41	14.039	2024	2032	2034	rVV2	1621187	1810785	39.87%	5.134%
42	14.063	2034	2036	2042	rVB	360936	313823	6.91%	0.890%
43	14.204	2057	2060	2063	rBV	70575	48610	1.07%	0.138%
44	14.421	2095	2097	2101	rVB	60145	56530	1.24%	0.160%
45	14.457	2101	2103	2107	rVB2	50012	53742	1.18%	0.152%
46	14.510	2107	2112	2116	rBV3	109166	144387	3.18%	0.409%
47	14.551	2116	2119	2121	rBV2	45023	55112	1.21%	0.156%
48	14.621	2129	2131	2137	rVB3	38587	48390	1.07%	0.137%
49	14.816	2161	2164	2167	rBV	63254	60112	1.32%	0.170%
50	15.080	2204	2209	2212	rBV	268278	403622	8.89%	1.144%
51	15.157	2219	2222	2225	rBV	85391	84597	1.86%	0.240%
52	15.186	2225	2227	2231	rVB	50510	51468	1.13%	0.146%
53	15.380	2257	2260	2266	rVB	141969	191500	4.22%	0.543%
54	15.445	2267	2271	2277	rBV	205638	251069	5.53%	0.712%
55	15.510	2277	2282	2286	rBV2	890850	1111752	24.48%	3.152%
56	15.980	2359	2362	2367	rVB2	42062	55830	1.23%	0.158%
57	16.221	2401	2403	2415	rVB10	34034	62965	1.39%	0.179%
58	16.980	2526	2532	2540	rVB2	78327	161998	3.57%	0.459%
59	17.421	2602	2607	2615	rVB2	53410	99699	2.20%	0.283%

Sum of corrected areas: 35271049

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Instrument :
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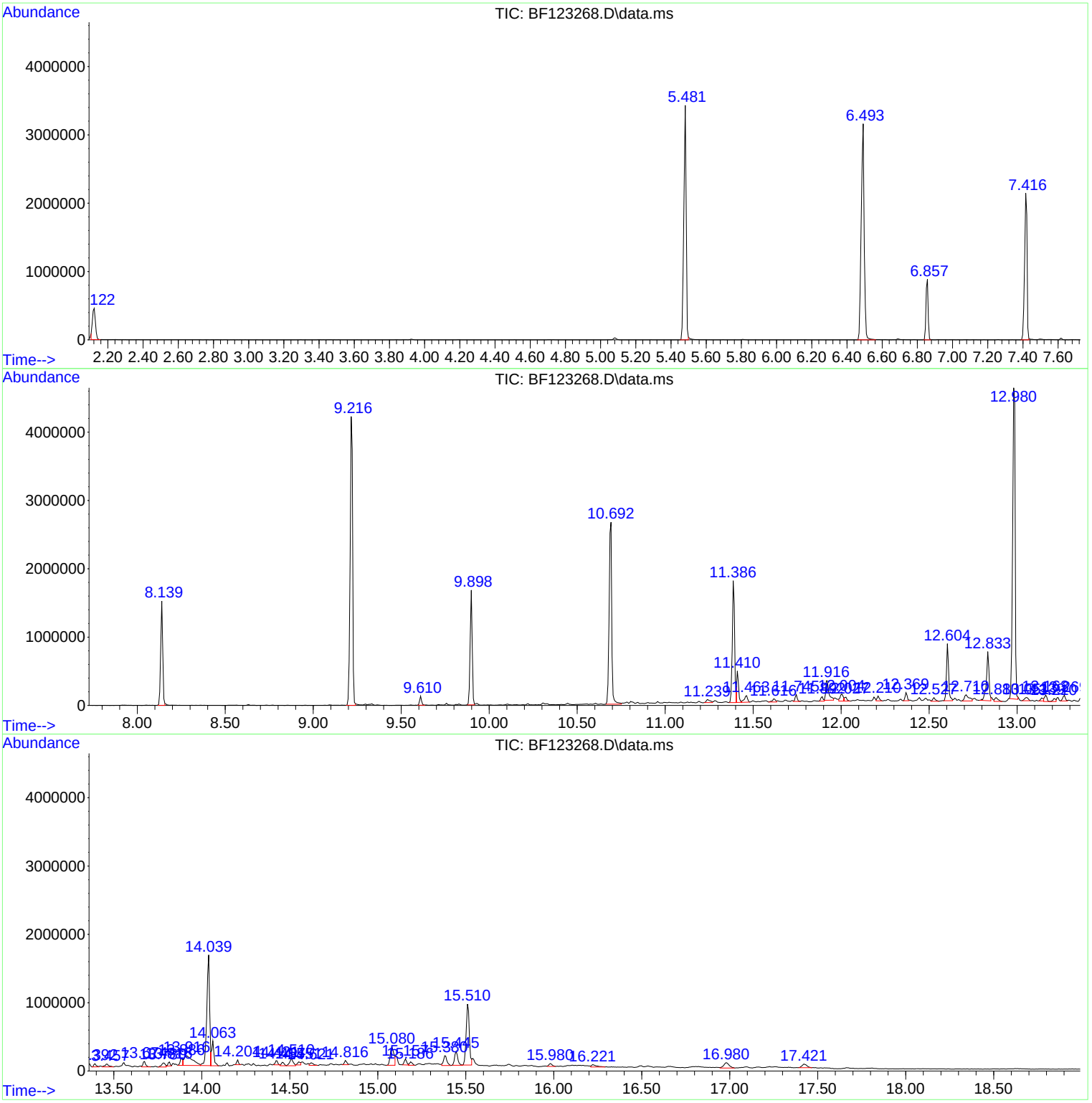
ClientSampleId :
TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.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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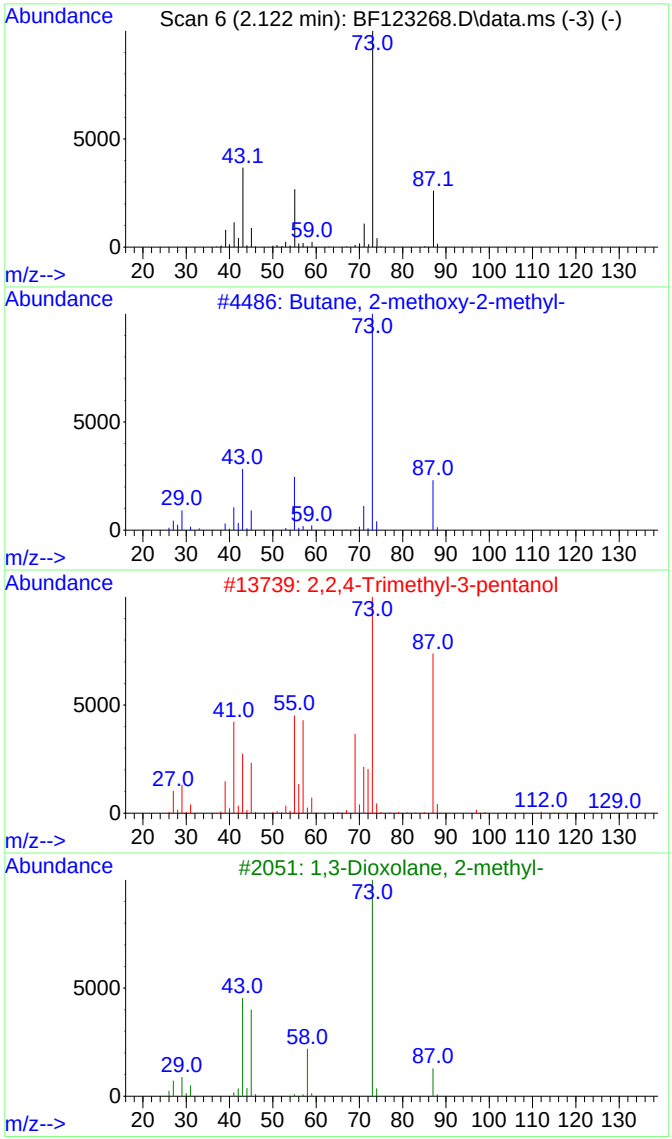
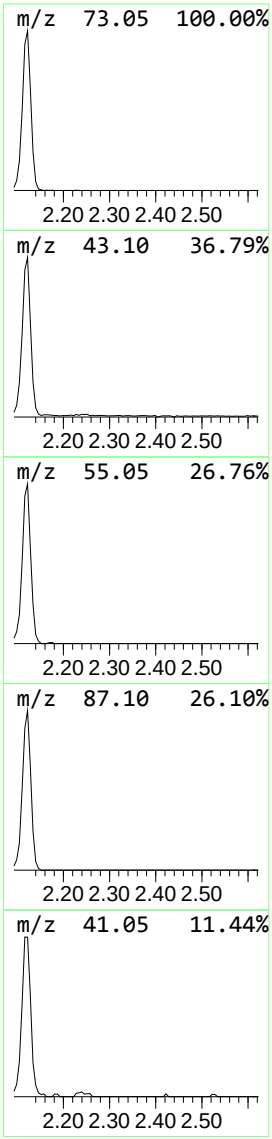
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	14.64 ng	542828	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.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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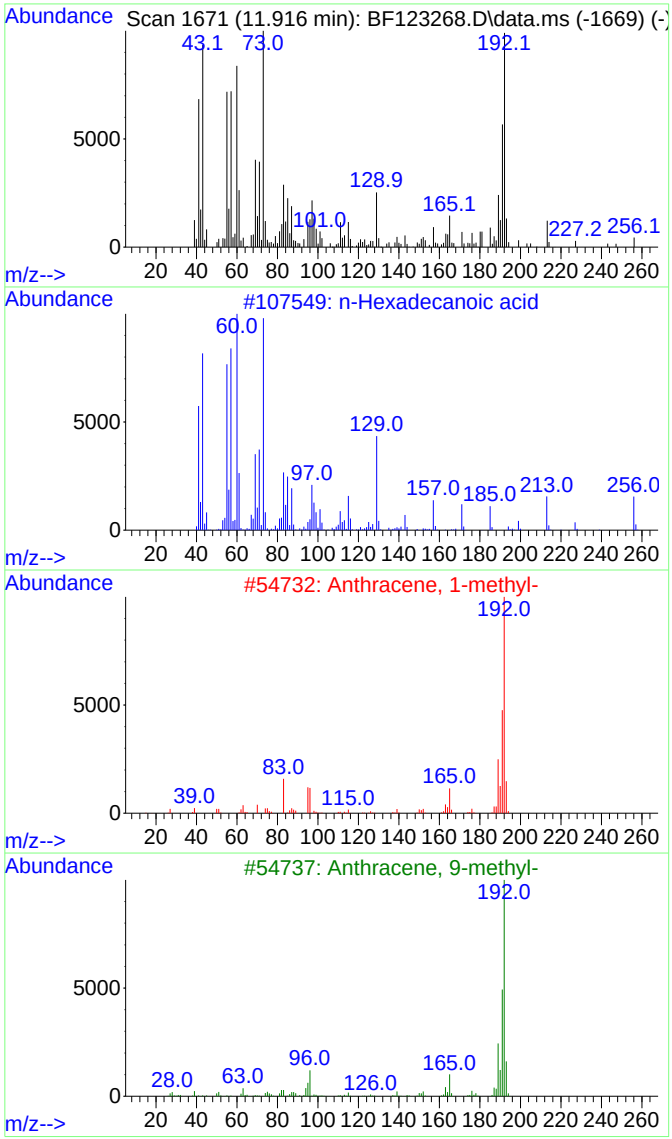
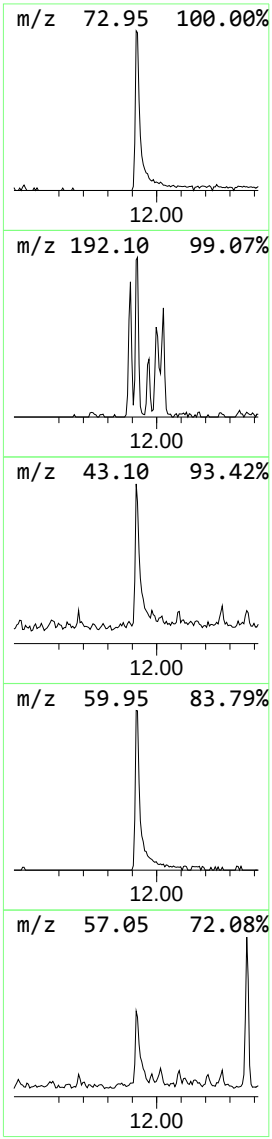
Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	4.30 ng	354874	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	64
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	64
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	64
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	62





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ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
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TIC Library : C:\DATABASE\NIST11.L
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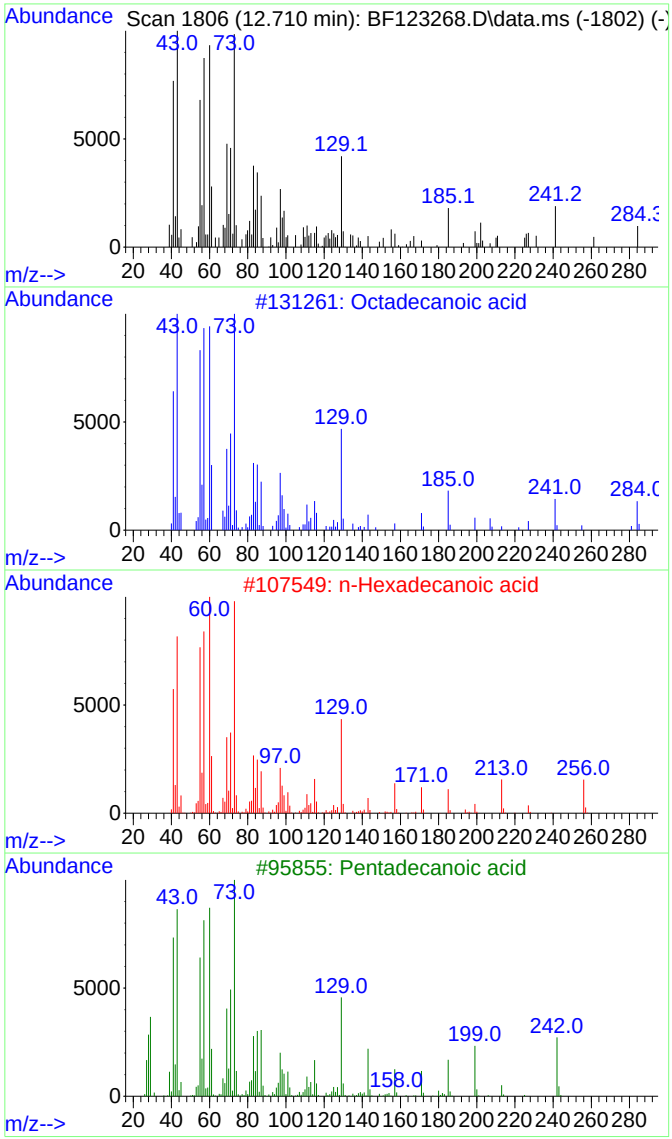
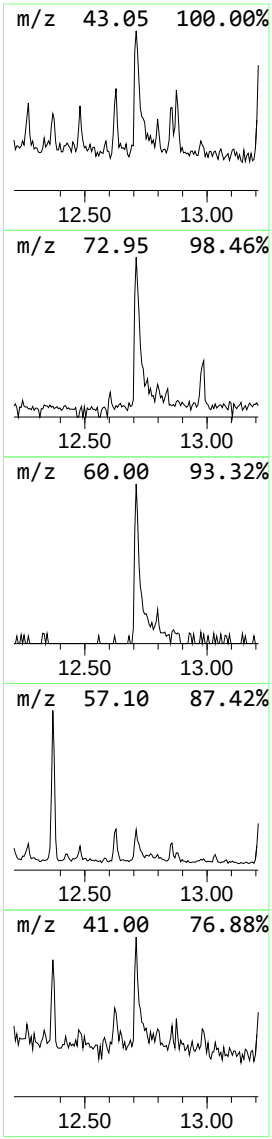
Peak Number 3 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.710	2.00 ng	165146	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Hexadecane	226	C16H34	000544-76-3	25
5	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	18





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

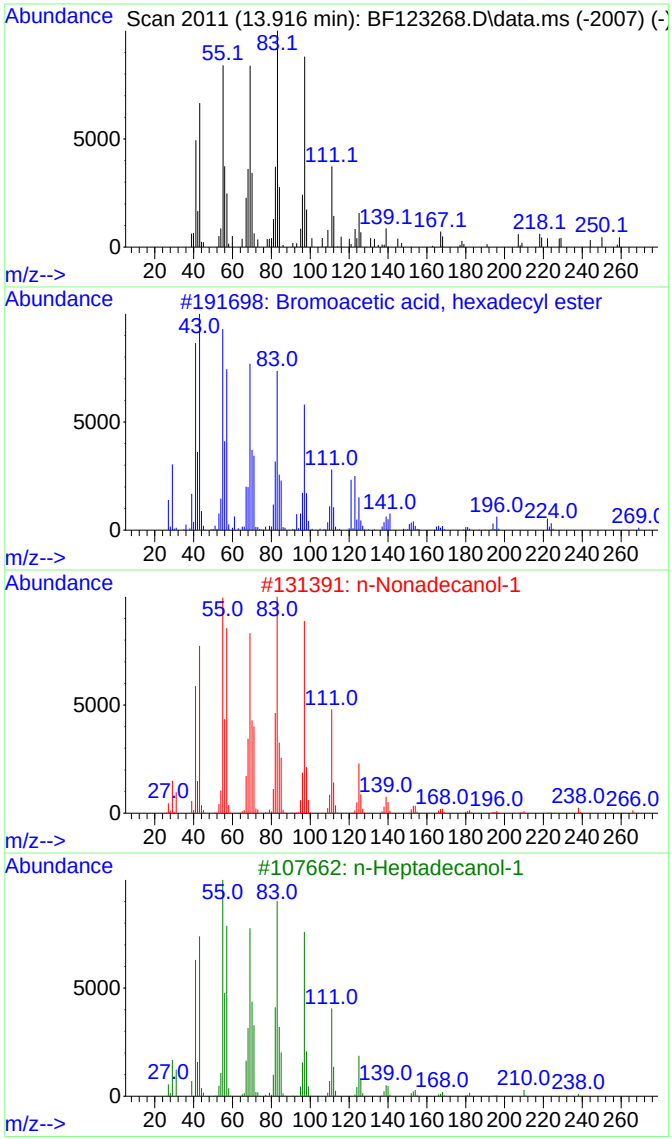
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

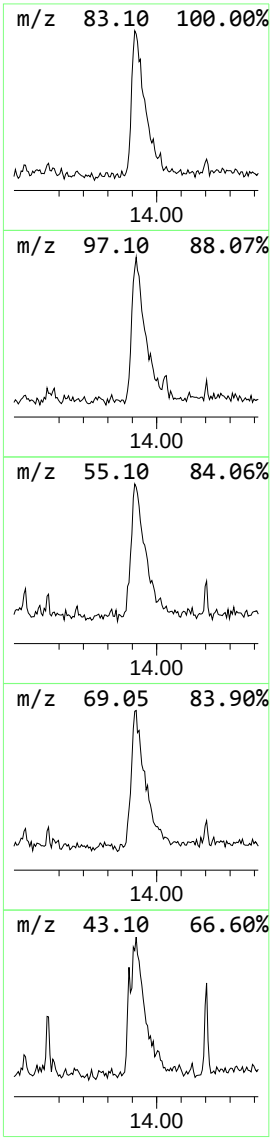
****

Peak Number 4 Bromoacetic acid, hexadecyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.916	5.27 ng	476840	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	90
3	n-Heptadecanol-1	256	C17H36O	001454-85-9	90
4	Isoheptadecanol	256	C17H36O	057289-07-3	72
5	1-Hexadecanol	242	C16H34O	036653-82-4	62





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Instrument :
BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

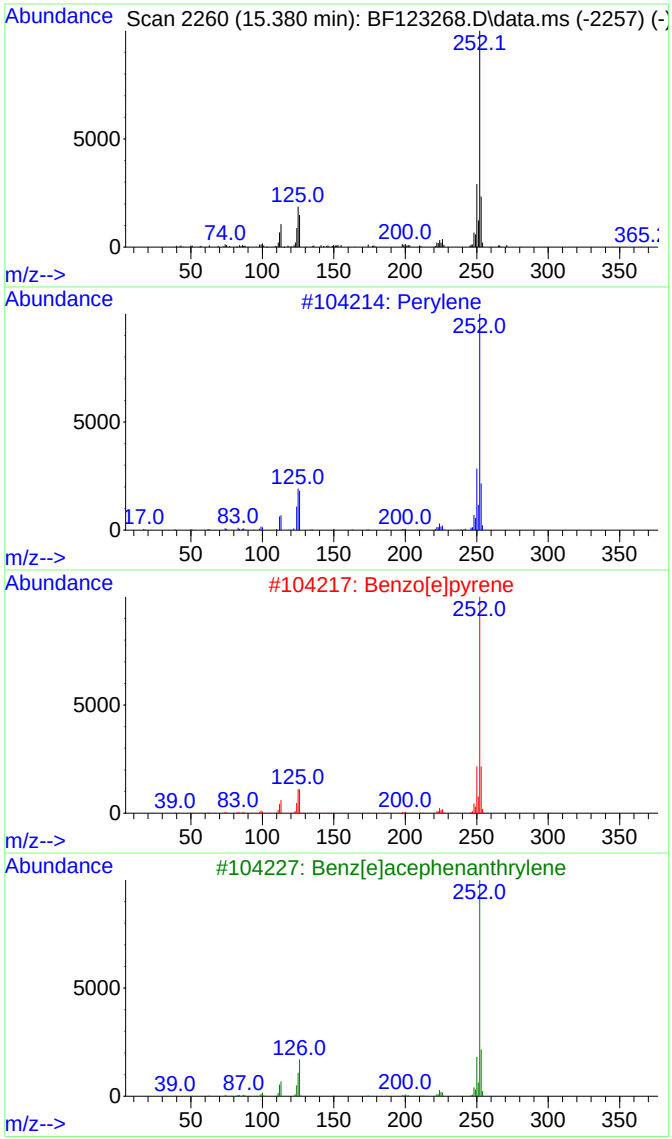
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

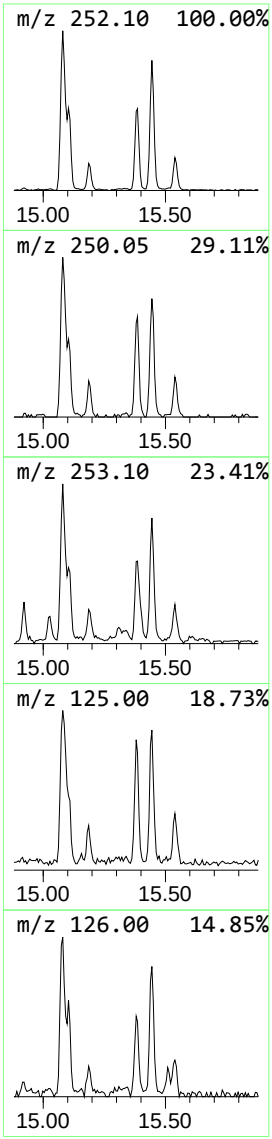
****

Peak Number 5 Perylene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.380	3.45 ng	191500	Perylene-d12	15.510

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	98
2	Benzo[e]pyrene	252	C20H12	000192-97-2	97
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	95
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93





Tentatively Identified Compound (LSC) summary

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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-metho...	2.122	14.6	ng	542828	1	6.857	741476	20.0
n-Hexadecanoic ...	11.916	4.3	ng	354874	4	11.386	1649440	20.0
Octadecanoic acid	12.710	2.0	ng	165146	4	11.386	1649440	20.0
Bromoacetic aci...	13.916	5.3	ng	476840	5	14.039	1810790	20.0
Perylene	15.380	3.5	ng	191500	6	15.510	1111750	20.0