LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020521\
Data File : BF123139.D
Acq On : 5 Feb 2021 17:12
Operator : JU/CG
Sample : M1315-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-1

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-BF012721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123139.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	6	13	18	rVB	392266	521563	9.66%	1.289%
2	5.110	502	514	524	rBV3	35887	88130	1.63%	0.218%
3	5.281	539	543	547	rBV	91797	95745	1.77%	0.237%
4	5.510	577	582	585	rBV	3724529	3625299	67.13%	8.958%
5	6.516	748	753	766	rBV	3505129	3773749	69.88%	9.324%
6	6.893	813	817	820	rBV	1297862	970164	17.97%	2.397%
7	7.451	907	912	915	rBV	2467782	2382379	44.12%	5.887%
8	8.175	1031	1035	1039	rBV	1473074	1276381	23.64%	3.154%
9	8.769	1132	1136	1139	rBV	168509	127369	2.36%	0.315%
10	9.257	1214	1219	1222	rBV	4931647	4353465	80.62%	10.757%
11	9.645	1282	1285	1289	rBV	84612	75117	1.39%	0.186%
12	9.939	1330	1335	1338	rBV	1665417	1529332	28.32%	3.779%
13	10.728	1465	1469	1480	rBV	2887588	2745078	50.83%	6.783%
14	11.428	1584	1588	1591	rBV	1854562	1717724	31.81%	4.244%
15	11.451	1591	1592	1595	rVB	309485	192181	3.56%	0.475%
16	11.963	1670	1679	1683	rBV	1353859	1356553	25.12%	3.352%
17	12.045	1691	1693	1702	rVB5	62298	93770	1.74%	0.232%
18	12.251	1726	1728	1732	rVB	114444	110884	2.05%	0.274%
19	12.416	1752	1756	1759	rBV	494008	445067	8.24%	1.100%
20	12.469	1762	1765	1770	rVB	112527	93649	1.73%	0.231%
21	12.645	1792	1795	1798	rBV	458979	402507	7.45%	0.995%
22	12.669	1798	1799	1805	rVB	96022	74342	1.38%	0.184%
23	12.751	1808	1813	1822	rBV	1572888	1689855	31.29%	4.175%
24	12.816	1822	1824	1827	rVV	146859	149274	2.76%	0.369%
25	12.875	1829	1834	1840	rVB	342183	429918	7.96%	1.062%
26	13.027	1855	1860	1863	rBV	5650897	5400243	100.00%	13.343%
27	13.174	1881	1885	1887	rBV	84659	108977	2.02%	0.269%
28	13.316	1905	1909	1911	rBV3	61036	66589	1.23%	0.165%
29	13.498	1937	1940	1946	rVV	163838	160209	2.97%	0.396%
30	13.551	1946	1949	1952	rVB	68327	65308	1.21%	0.161%
31	13.645	1961	1965	1968	rBV	566725	500922	9.28%	1.238%
32	13.674	1968	1970	1973	rVV2	85353	77706	1.44%	0.192%
33	13.722	1975	1978	1983	rVB2	75772	81173	1.50%	0.201%
34	13.874	1999	2004	2010	rVB5	83826	160963	2.98%	0.398%
35	13.927	2010	2013	2018	rVB2	65030	82810	1.53%	0.205%
36	14.033	2023	2031	2035	rVV7	219129	622511	11.53%	1.538%

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.080	2035	2039	2042	rVV	1979986	2063021	38.20%	5.097%
38	14.104	2042	2043	2050	rVB	194309	175875	3.26%	0.435%
39	14.551	2117	2119	2124	rVB3	59438	67634	1.25%	0.167%
40	14.716	2144	2147	2151	rBV	161702	144969	2.68%	0.358%
41	14.868	2170	2173	2178	rVB	59388	62677	1.16%	0.155%
42	14.945	2184	2186	2189	rBV	75962	79500	1.47%	0.196%
43	15.016	2195	2198	2201	rVB	129275	117894	2.18%	0.291%
44	15.133	2214	2218	2222	rBV	133326	214585	3.97%	0.530%
45	15.216	2229	2232	2235	rVB	80360	75652	1.40%	0.187%
46	15.445	2268	2271	2278	rVB	89859	135386	2.51%	0.335%
47	15.504	2278	2281	2287	rVB	85650	101863	1.89%	0.252%
48	15.574	2288	2293	2297	rBV	1097542	1452881	26.90%	3.590%
49	16.057	2371	2375	2380	rVB	91040	133035	2.46%	0.329%

Sum of corrected areas: 40471878

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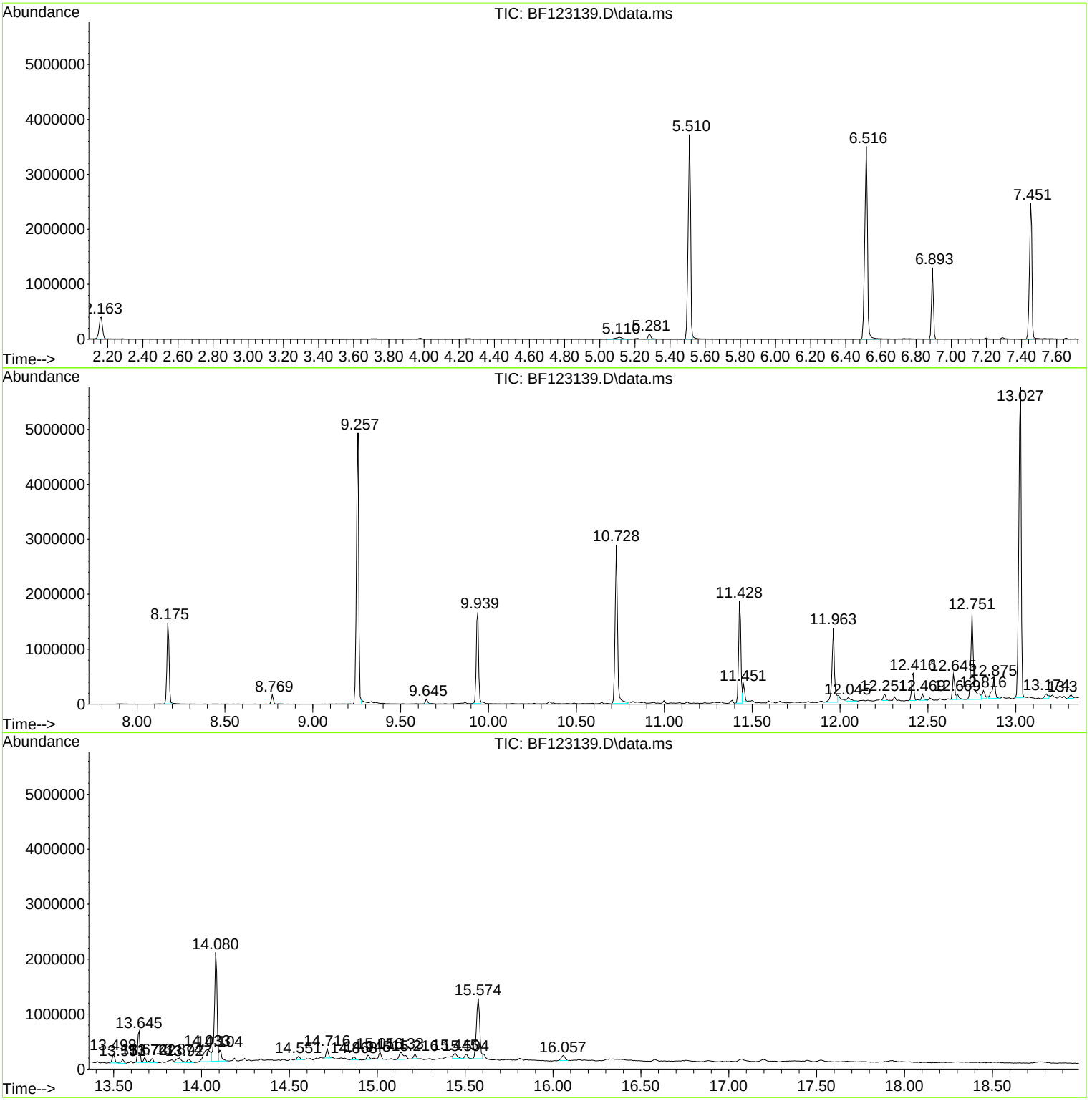
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Sample : M1315-04
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Instrument : BNA_F
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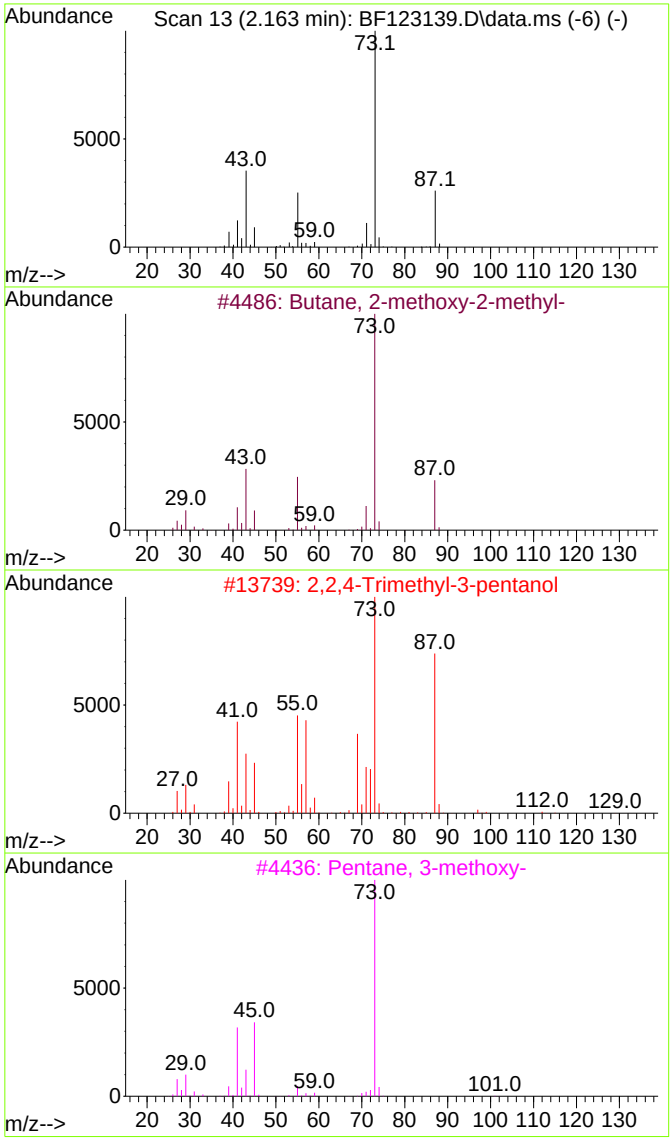
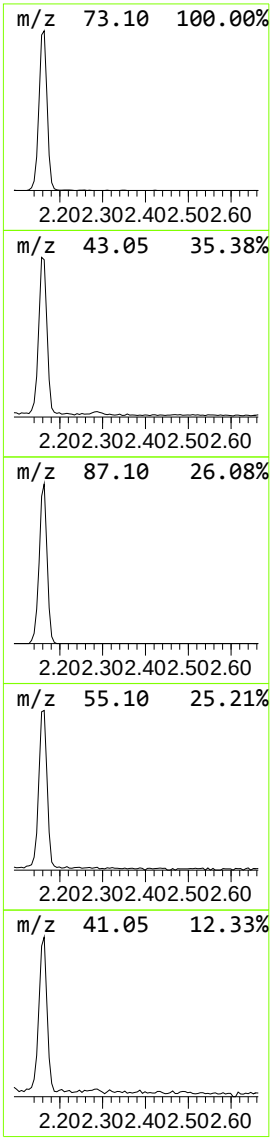
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	10.75 ng	521563	1,4-Dichlorobenzene-d4	6.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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Sample : M1315-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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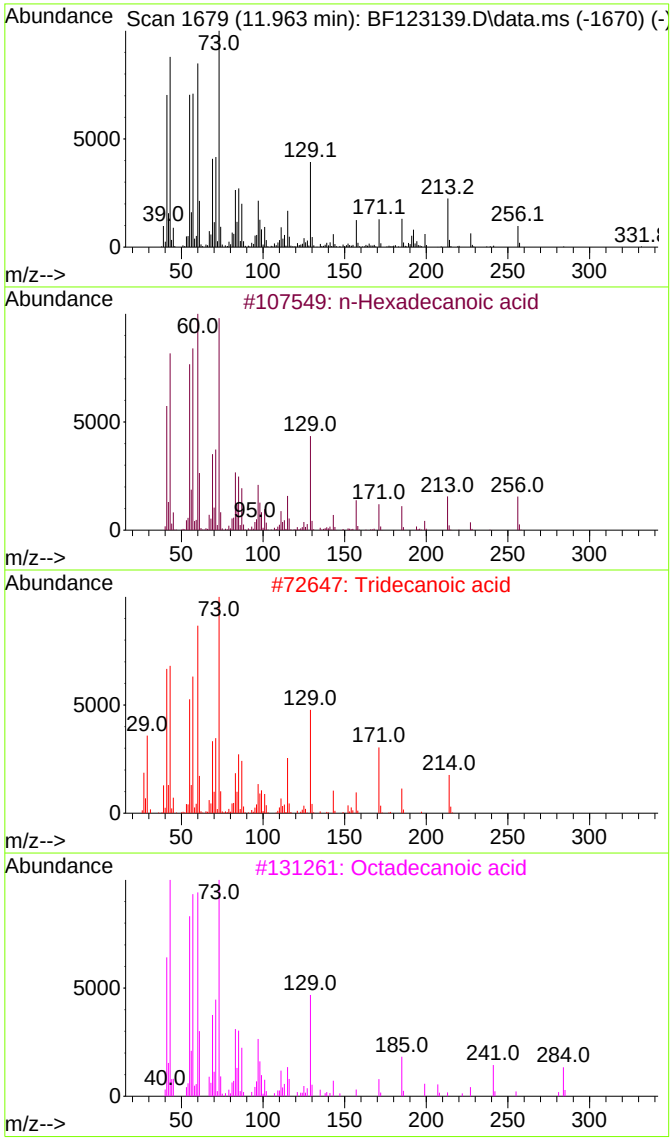
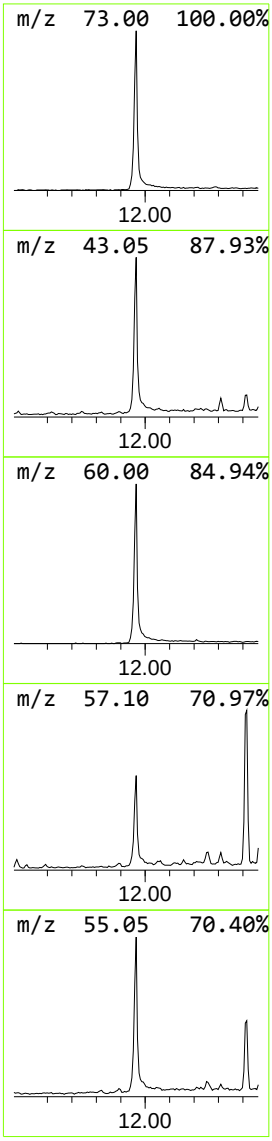
Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.963	15.79 ng	1356550	Phenanthrene-d10	11.428

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Octadecanoic acid	284	C18H36O2	000057-11-4	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	91





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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
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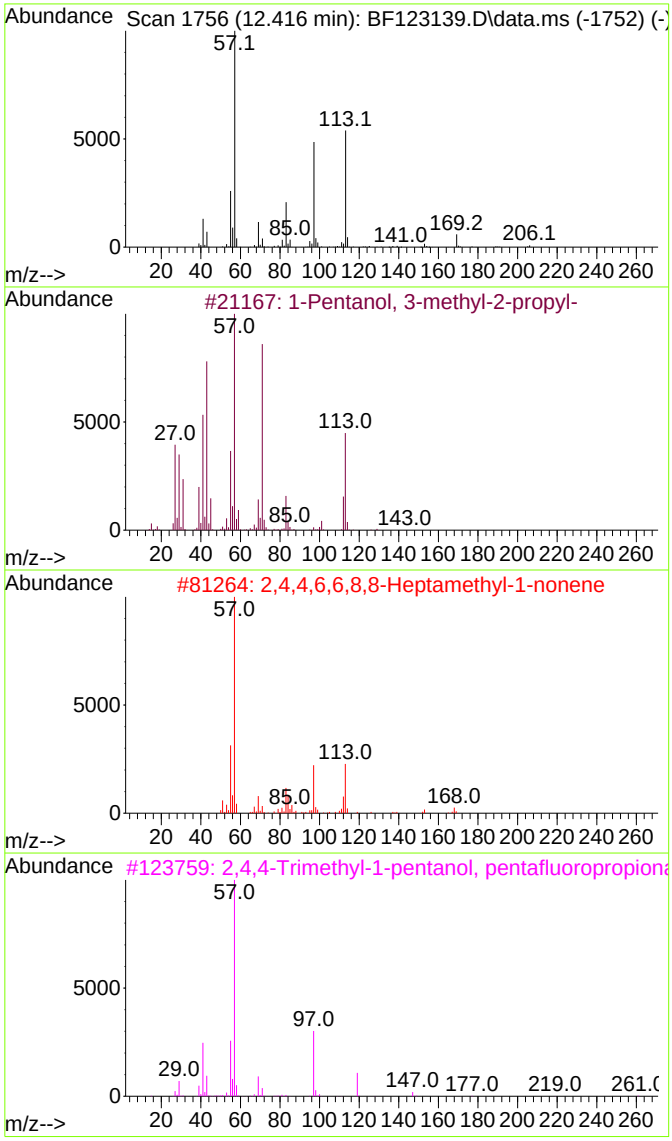
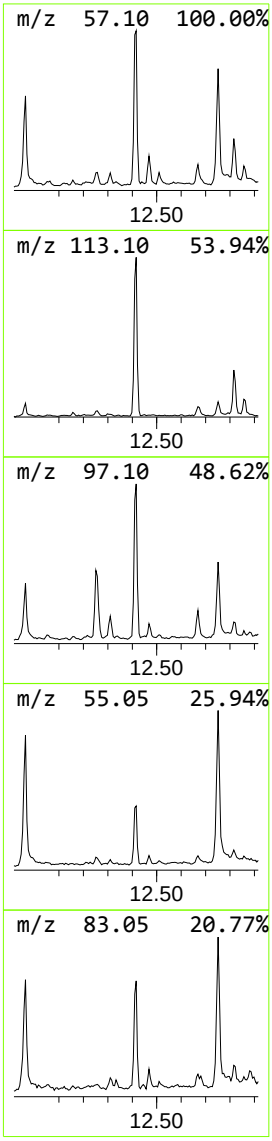
Peak Number 3 unknown12.14 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.416	5.18 ng	445067	Phenanthrene-d10	11.428

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	38
2	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	37
3	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	32
4	Pyrazole, 3-nitro-	113	C3H3N3O2	026621-44-3	25
5	Hexanal, 3,5,5-trimethyl-	142	C9H18O	005435-64-3	22





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ALS Vial : 13 Sample Multiplier: 1

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

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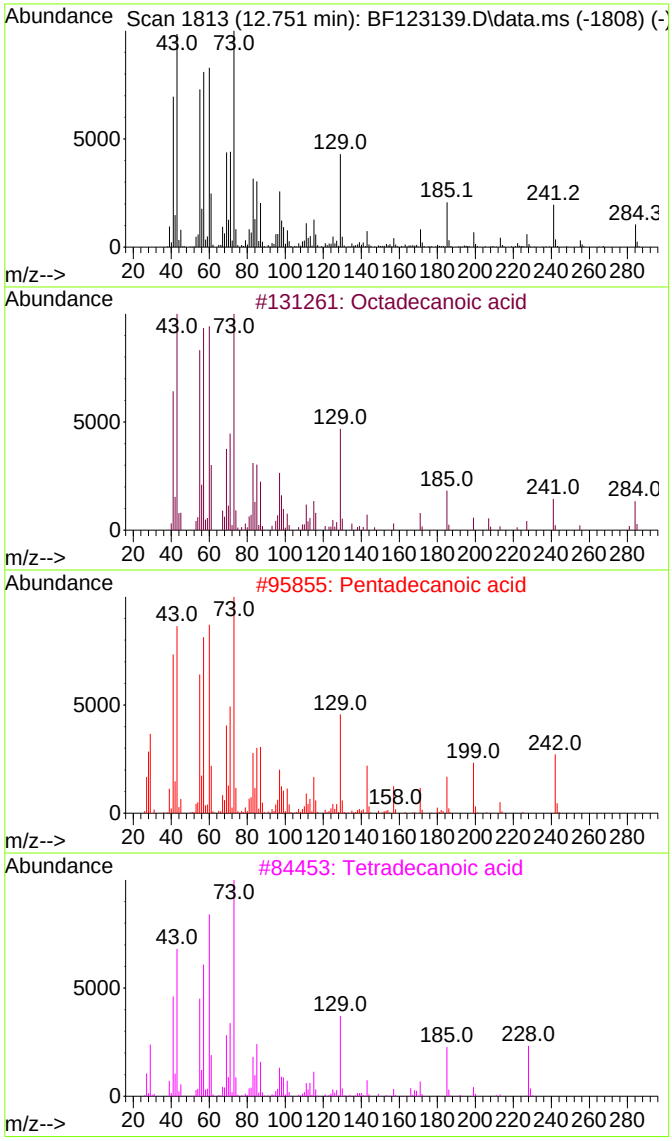
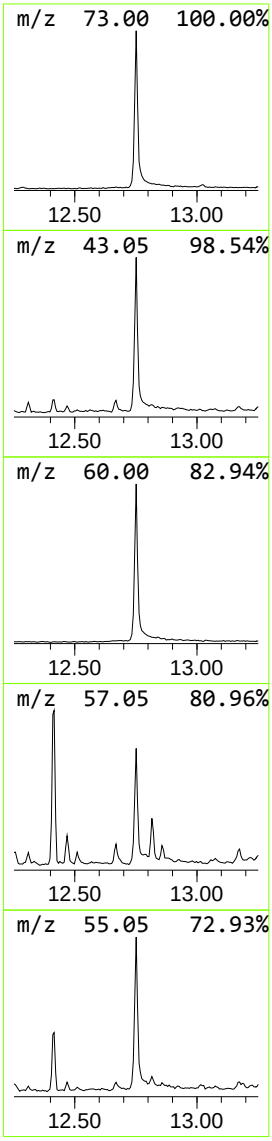
Peak Number 4 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.751	19.68 ng	1689860	Phenanthrene-d10	11.428

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	74
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62





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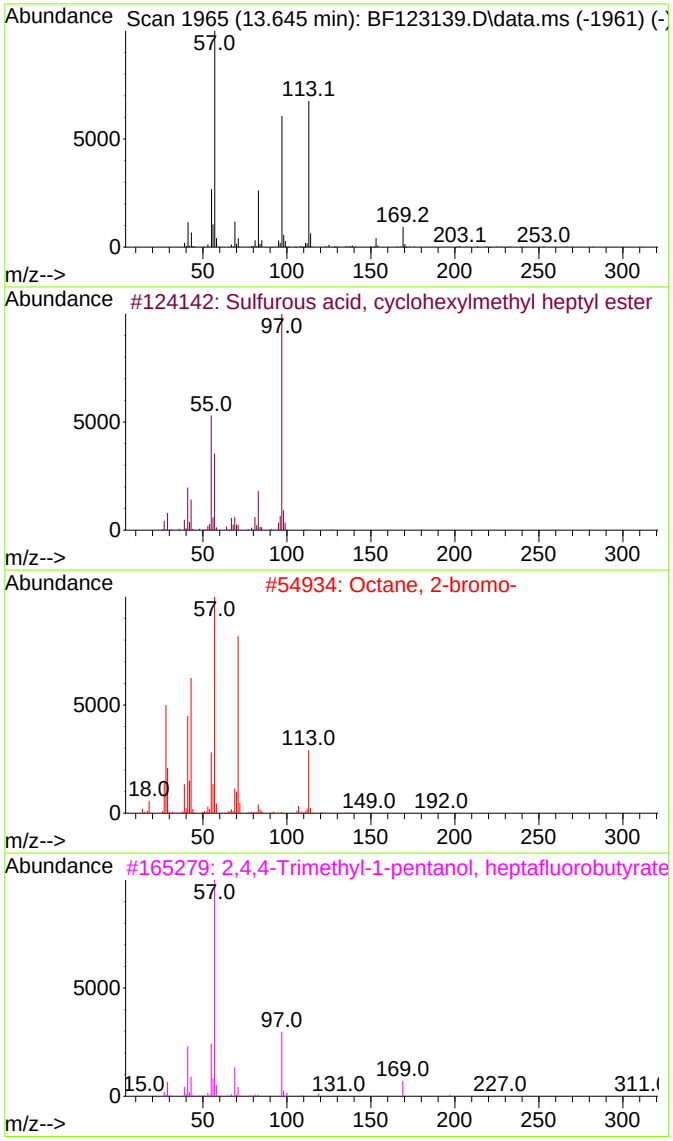
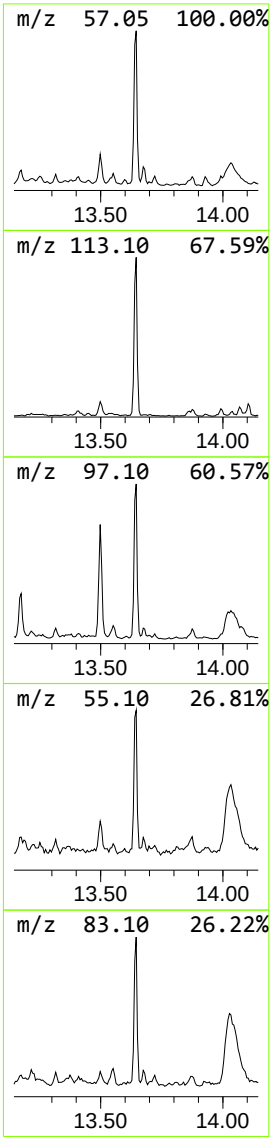
Peak Number 5 unknown13.64 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.645	4.86 ng	500922	Chrysene-d12	14.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	32
2	Octane, 2-bromo-	192	C8H17Br	000557-35-7	32
3	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	27
4	Cyclohexane, (bromomethyl)-	176	C7H13Br	002550-36-9	27
5	Sulfurous acid, cyclohexylmethyl...	402	C23H46O3S	1000309-22-4	25





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.163	10.8	ng	521563	1	6.893	970164	20.0
n-Hexadecanoic ...	11.963	15.8	ng	1356550	4	11.428	1717720	20.0
unknown12.14	12.416	5.2	ng	445067	4	11.428	1717720	20.0
Octadecanoic acid	12.751	19.7	ng	1689860	4	11.428	1717720	20.0
unknown13.64	13.645	4.9	ng	500922	5	14.080	2063020	20.0