LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030419\
Data File : BF112823.D
Acq On : 4 Mar 2019 14:45
Operator : JU/SJ
Sample : K1707-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12

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-BF022719.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	3.746	275	282	288	rBV	23599	38350	1.04%	0.097%
2	4.440	397	400	404	rBV	33893	38805	1.05%	0.098%
3	5.357	551	556	559	rBV	3461182	3272033	88.35%	8.272%
4	6.287	710	714	719	rVB2	38717	46018	1.24%	0.116%
5	6.381	725	730	733	rBV	3609430	3625808	97.90%	9.166%
6	6.516	748	753	756	rBV	4012039	3703516	100.00%	9.362%
7	6.745	788	792	795	rBV	1205261	950067	25.65%	2.402%
8	6.904	815	819	822	rBV	3099604	2878875	77.73%	7.278%
9	7.145	856	860	863	rBV2	47797	48646	1.31%	0.123%
10	7.304	882	887	890	rBV	2578454	2419847	65.34%	6.117%
11	8.028	1006	1010	1012	rBV	1180526	1142591	30.85%	2.888%
12	8.045	1012	1013	1021	rVB2	151660	166371	4.49%	0.421%
13	8.463	1081	1084	1087	rBV	67108	52899	1.43%	0.134%
14	8.628	1109	1112	1117	rBV	43043	42034	1.13%	0.106%
15	8.739	1125	1131	1136	rVB	94699	100326	2.71%	0.254%
16	8.833	1144	1147	1151	rBV	55644	51375	1.39%	0.130%
17	9.098	1188	1192	1203	rBV	3813801	3605697	97.36%	9.115%
18	9.192	1206	1208	1212	rVB2	74478	77491	2.09%	0.196%
19	9.433	1247	1249	1252	rBV	41540	43418	1.17%	0.110%
20	9.492	1256	1259	1261	rBV	248278	213230	5.76%	0.539%
21	9.633	1279	1283	1286	rBV	48371	50918	1.37%	0.129%
22	9.722	1295	1298	1302	rVB	62397	52963	1.43%	0.134%
23	9.775	1302	1307	1311	rBV	1372301	1279491	34.55%	3.235%
24	9.804	1311	1312	1316	rVB2	49960	40634	1.10%	0.103%
25	9.980	1338	1342	1345	rBV	66210	60266	1.63%	0.152%
26	10.216	1380	1382	1386	rVB2	54043	48348	1.31%	0.122%
27	10.439	1416	1420	1423	rBV2	34833	40094	1.08%	0.101%
28	10.475	1423	1426	1432	rVB5	27423	44944	1.21%	0.114%
29	10.557	1436	1440	1452	rVV	2356627	2228525	60.17%	5.634%
30	10.686	1459	1462	1469	rBV2	86965	127063	3.43%	0.321%
31	11.057	1522	1525	1530	rVB3	40190	47160	1.27%	0.119%
32	11.133	1536	1538	1542	rBV3	60701	57297	1.55%	0.145%
33	11.251	1554	1558	1561	rBV	1300382	1169566	31.58%	2.957%
34	11.274	1561	1562	1566	rVV	311346	183020	4.94%	0.463%

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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.322	1568	1570	1574	rVB	54868	52318	1.41%	0.132%
36	11.363	1574	1577	1581	rBV4	36376	45689	1.23%	0.116%
37	11.751	1640	1643	1645	rBV	73898	66846	1.80%	0.169%
38	11.786	1645	1649	1654	rVV2	541010	651521	17.59%	1.647%
39	11.863	1658	1662	1664	rVV	129198	151019	4.08%	0.382%
40	11.886	1664	1666	1672	rVB	69930	63973	1.73%	0.162%
41	11.963	1677	1679	1682	rBV	55286	51637	1.39%	0.131%
42	12.045	1691	1693	1695	rBV	65921	59355	1.60%	0.150%
43	12.180	1713	1716	1717	rBV	41217	41087	1.11%	0.104%
44	12.304	1733	1737	1739	rBV	104283	109663	2.96%	0.277%
45	12.357	1744	1746	1748	rVB	85754	68686	1.85%	0.174%
46	12.386	1748	1751	1756	rBV3	40584	57281	1.55%	0.145%
47	12.457	1760	1763	1767	rBV	424966	389703	10.52%	0.985%
48	12.510	1769	1772	1777	rVB2	57046	72259	1.95%	0.183%
49	12.568	1779	1782	1789	rBV2	192887	219334	5.92%	0.554%
50	12.686	1797	1802	1805	rBV	392231	384144	10.37%	0.971%
51	12.727	1805	1809	1810	rVV2	37795	42590	1.15%	0.108%
52	12.833	1823	1827	1830	rBV	2900030	2500961	67.53%	6.322%
53	12.904	1836	1839	1842	rBV2	67023	70025	1.89%	0.177%
54	13.016	1856	1858	1861	rVB	77994	69282	1.87%	0.175%
55	13.080	1866	1869	1872	rVB	113125	95460	2.58%	0.241%
56	13.116	1872	1875	1878	rBV	73417	73560	1.99%	0.186%
57	13.210	1888	1891	1894	rBV	55629	45420	1.23%	0.115%
58	13.239	1894	1896	1901	rVB	57584	53254	1.44%	0.135%
59	13.421	1924	1927	1933	rVB2	115260	129393	3.49%	0.327%
60	13.515	1941	1943	1949	rVB	82168	109242	2.95%	0.276%
61	13.627	1958	1962	1965	rBV2	69861	91914	2.48%	0.232%
62	13.739	1977	1981	1988	rVB3	452408	577870	15.60%	1.461%
63	13.880	2000	2005	2007	rBV2	1247579	1393748	37.63%	3.523%
64	13.904	2007	2009	2011	rVB	227217	171902	4.64%	0.435%
65	14.063	2033	2036	2039	rVB3	174217	159624	4.31%	0.404%
66	14.262	2066	2070	2073	rBV	102014	127656	3.45%	0.323%
67	14.298	2074	2076	2079	rVB	76328	65503	1.77%	0.166%
68	14.368	2085	2088	2090	rBV	178048	152737	4.12%	0.386%
69	14.662	2135	2138	2144	rVB2	234504	269273	7.27%	0.681%
70	14.892	2173	2177	2180	rBV	239015	355131	9.59%	0.898%
71	14.986	2189	2193	2199	rVB2	241225	313998	8.48%	0.794%

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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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72	15.174	2222	2225	2230	rVB	148629	168878	4.56%	0.427%
73	15.227	2231	2234	2240	rVV	209835	245246	6.62%	0.620%
74	15.292	2240	2245	2249	rVV	878262	1055789	28.51%	2.669%
75	15.339	2251	2253	2258	rVB	195038	239087	6.46%	0.604%
76	15.751	2319	2323	2326	rBV	138598	193895	5.24%	0.490%
77	15.792	2327	2330	2339	rVB6	113153	206553	5.58%	0.522%
78	16.651	2473	2476	2484	rVB2	82007	147312	3.98%	0.372%

Sum of corrected areas: 39557504

LSC Report - Integrated Chromatogram

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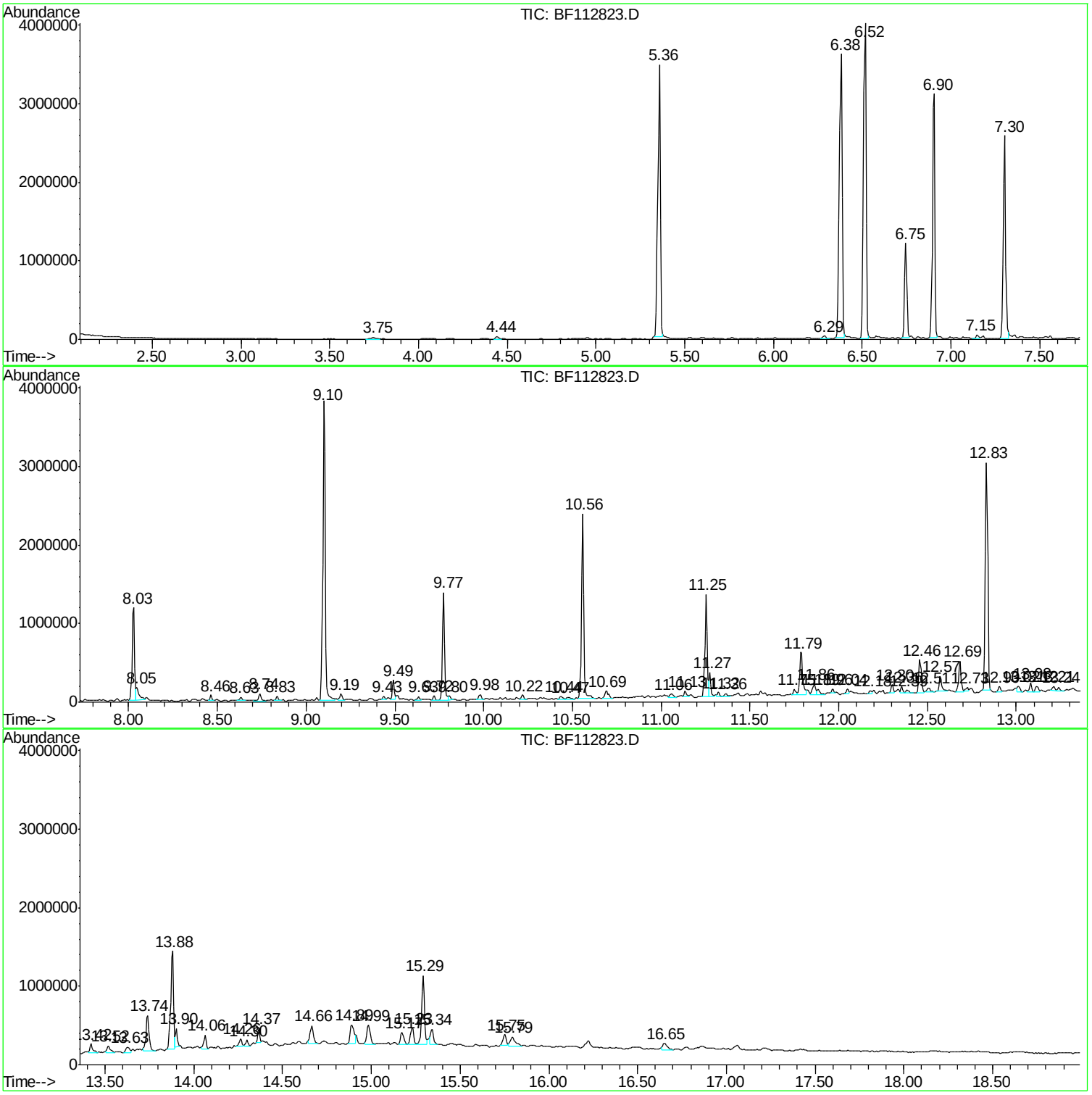
Sample : K1707-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
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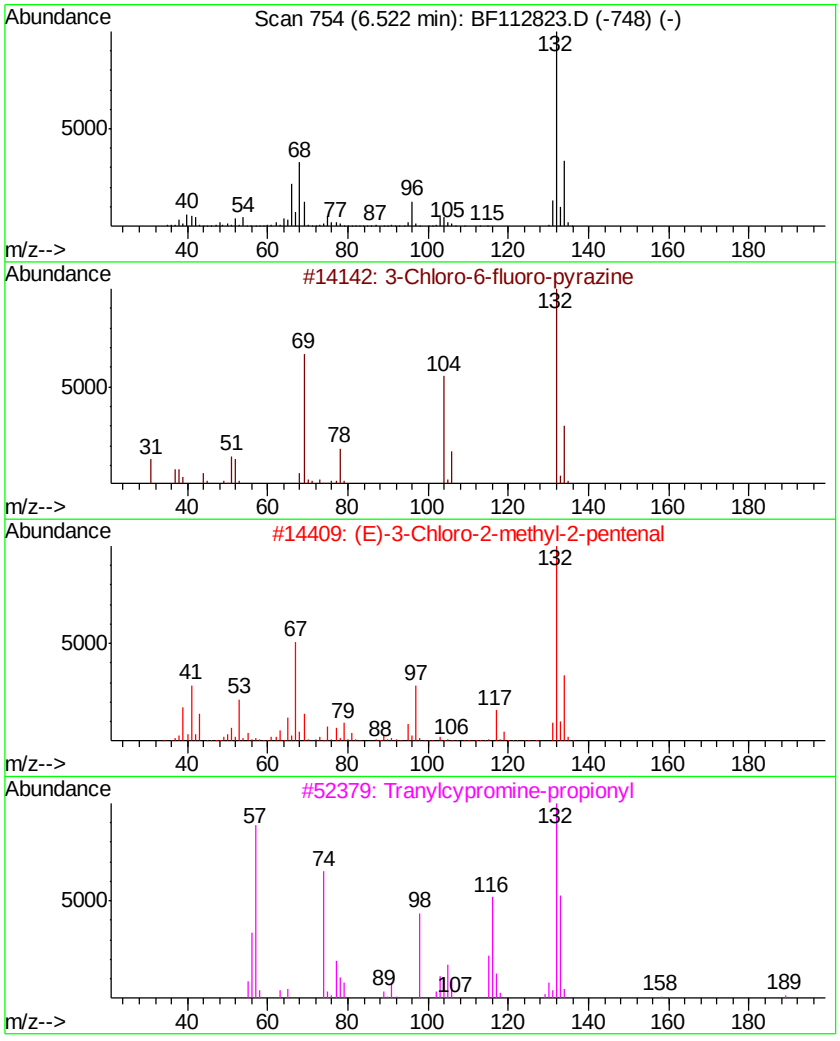
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

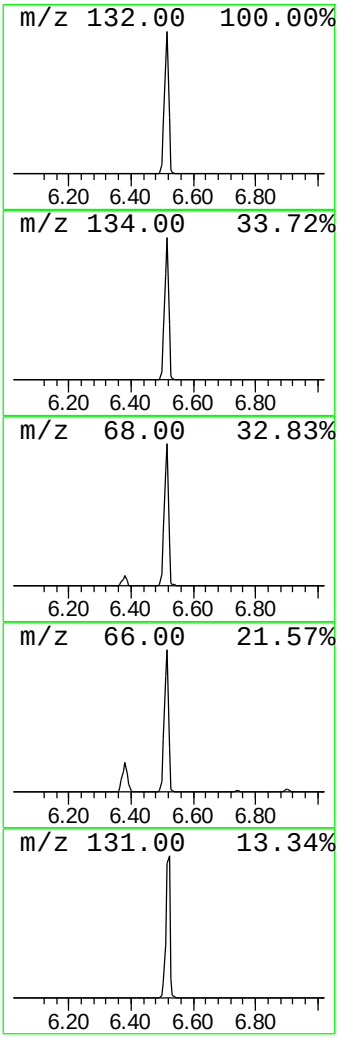
****

Peak Number 1 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	77.96 ng	3703520	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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

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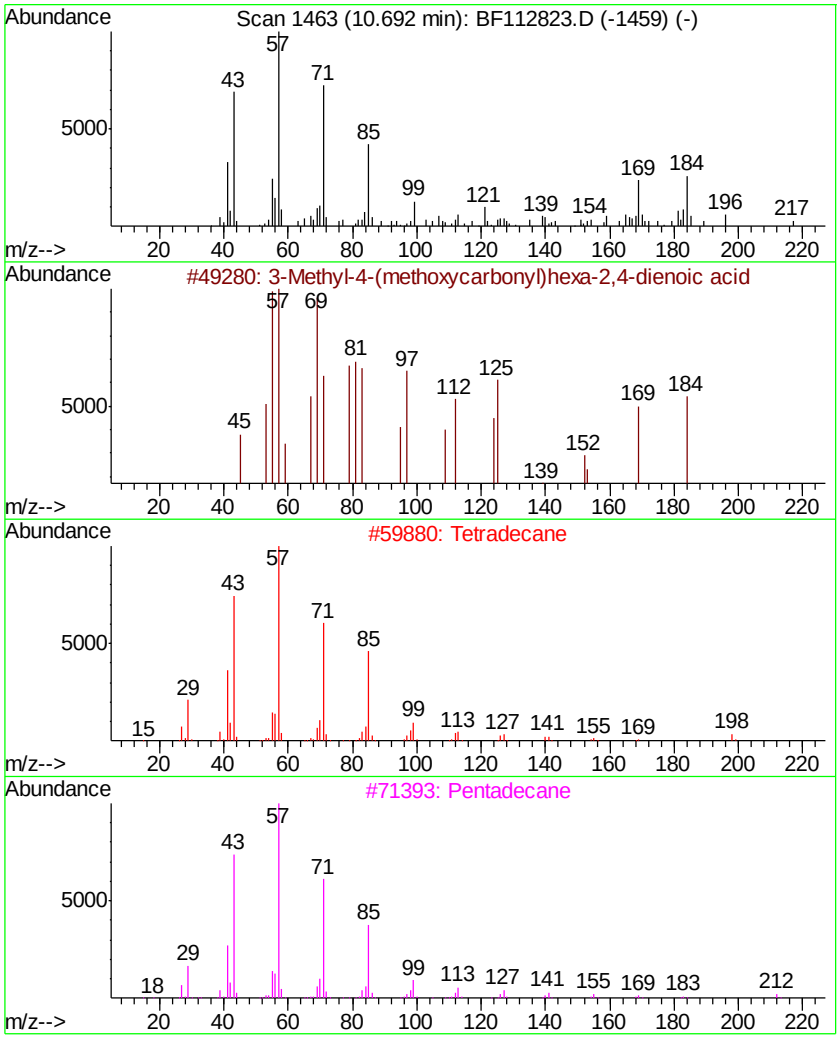
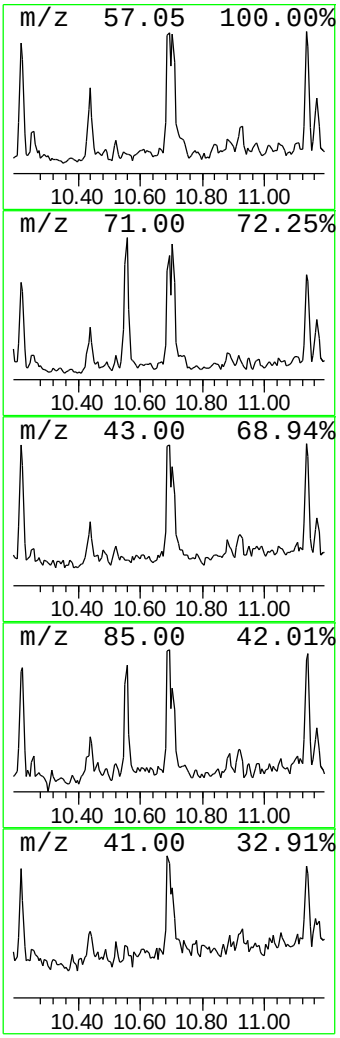
Peak Number 3 3-Methyl-4-(methoxycarbonyl... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.69	2.17 ng	127063	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methyl-4-(methoxycarbonyl)hexa...	184	C9H12O4	1000104-10-8	70
2	Tetradecane	198	C14H30	000629-59-4	50
3	Pentadecane	212	C15H32	000629-62-9	38
4	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	38
5	Dodecane	170	C12H26	000112-40-3	38





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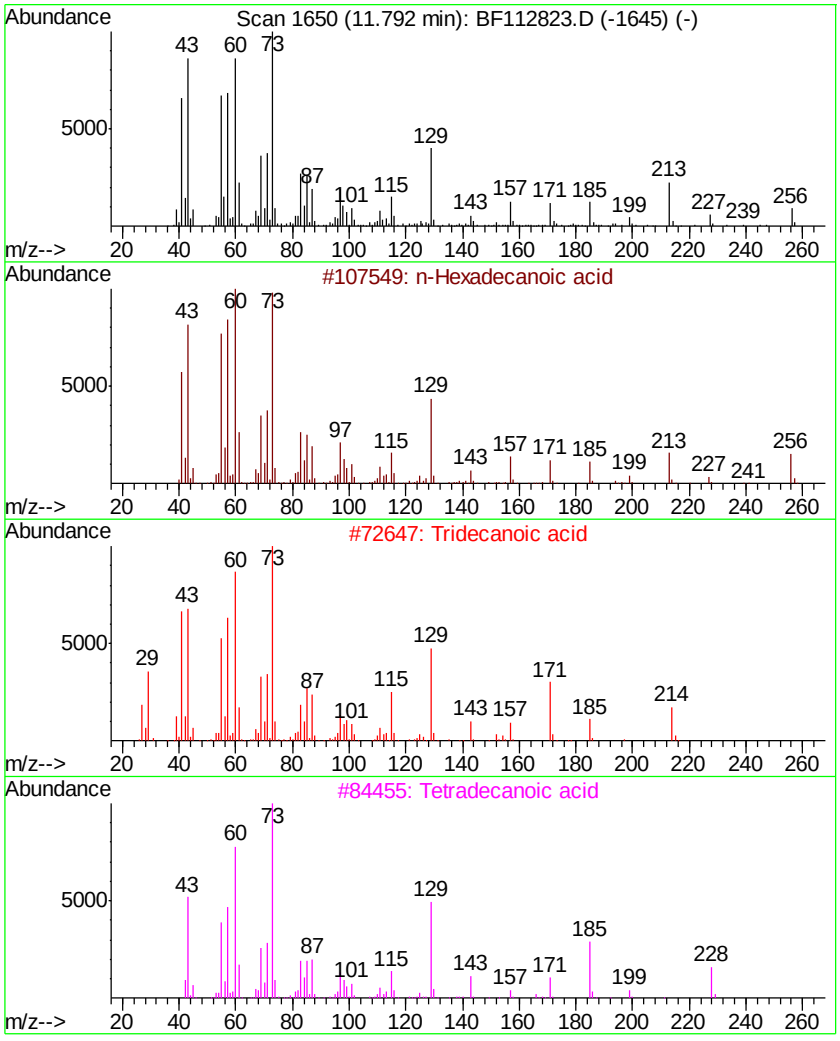
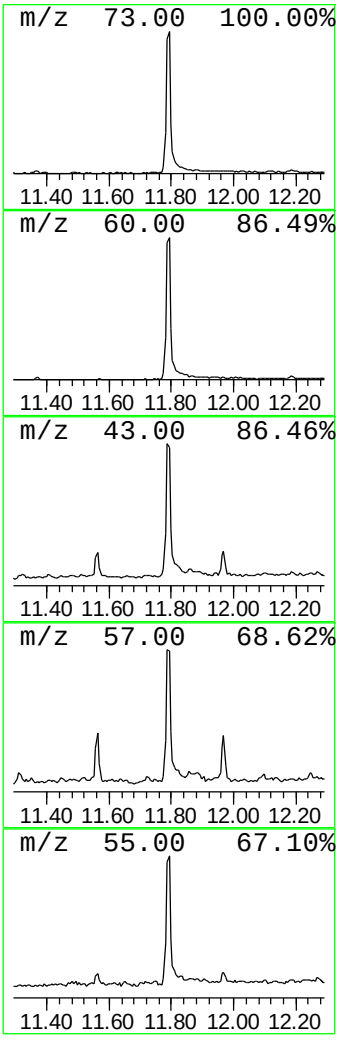
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	11.14 ng	651521	Phenanthrene-d10	11.25

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	96
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
5	Octanoic acid	144	C8H16O2	000124-07-2	38





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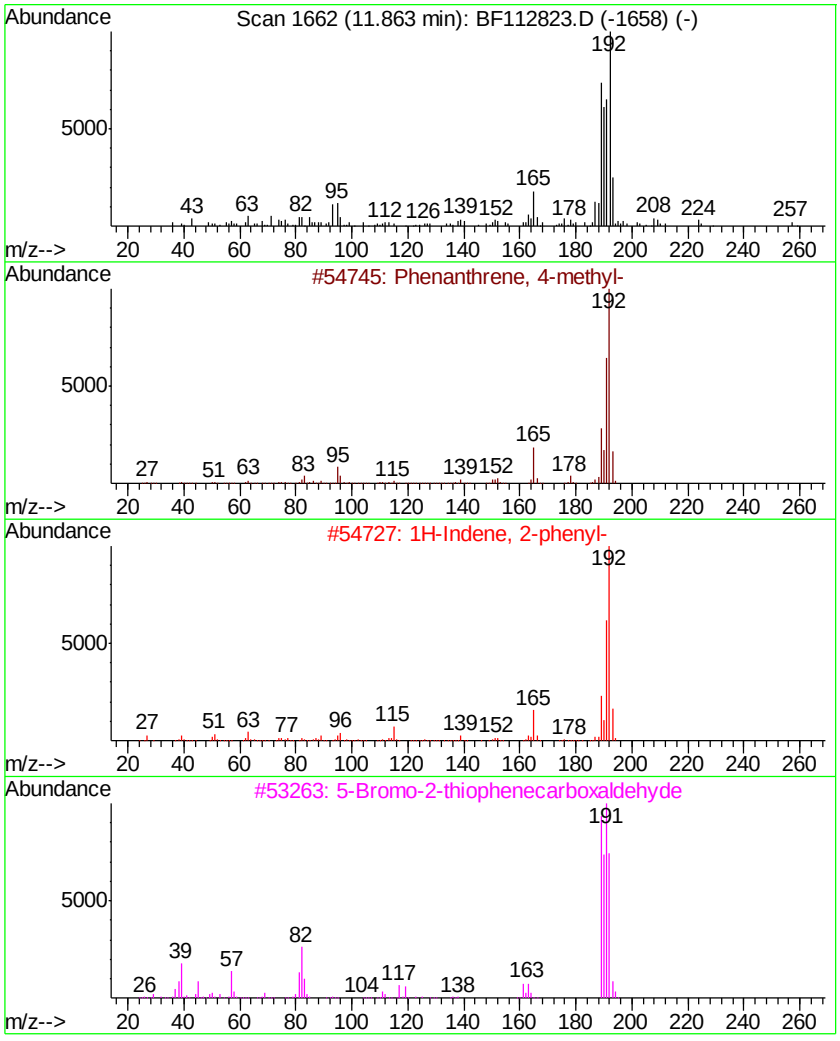
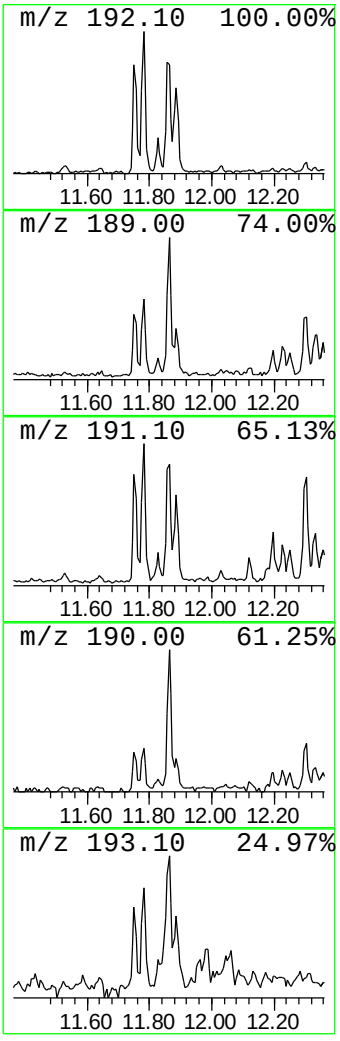
Peak Number 5 Phenanthrene, 4-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	2.58 ng	151019	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	64
2	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	55
3	5-Bromo-2-thiophenecarboxaldehyde	190	C5H3BrOS	004701-17-1	52
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	50
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	50





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

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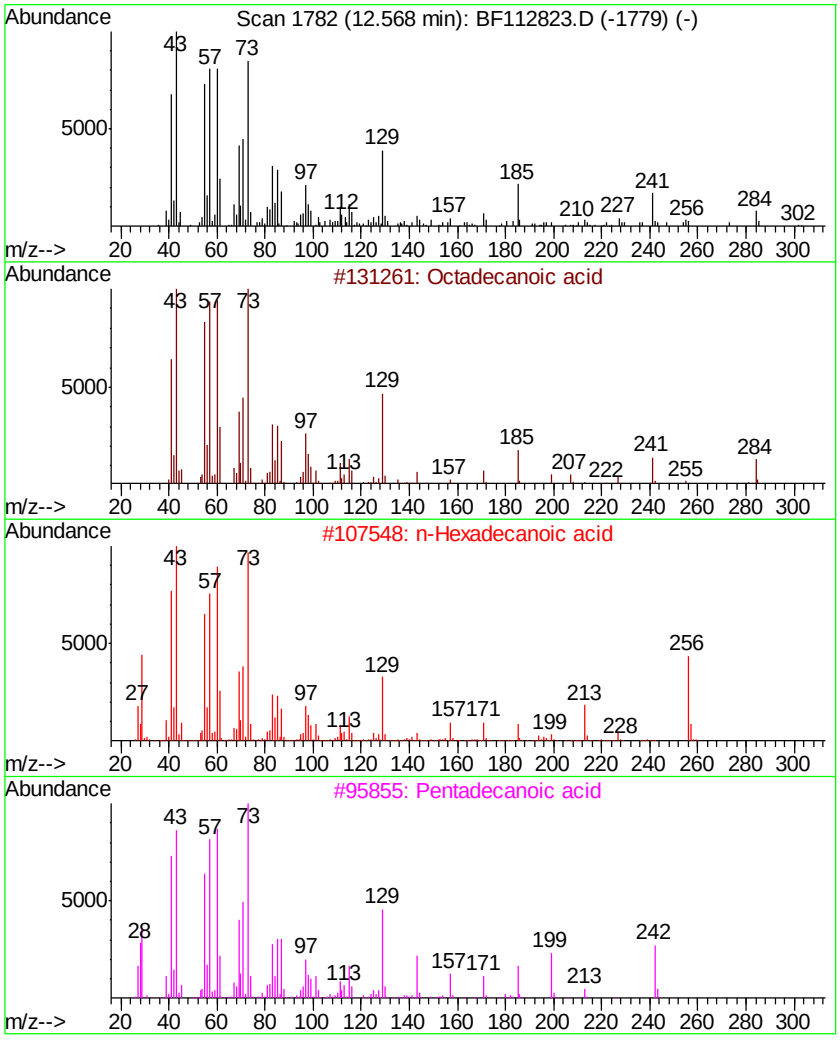
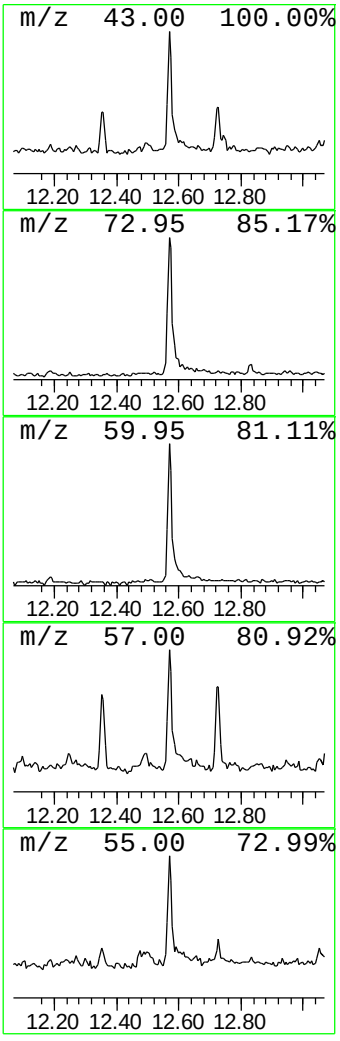
Peak Number 6 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	3.15 ng	219334	Chrysene-d12	13.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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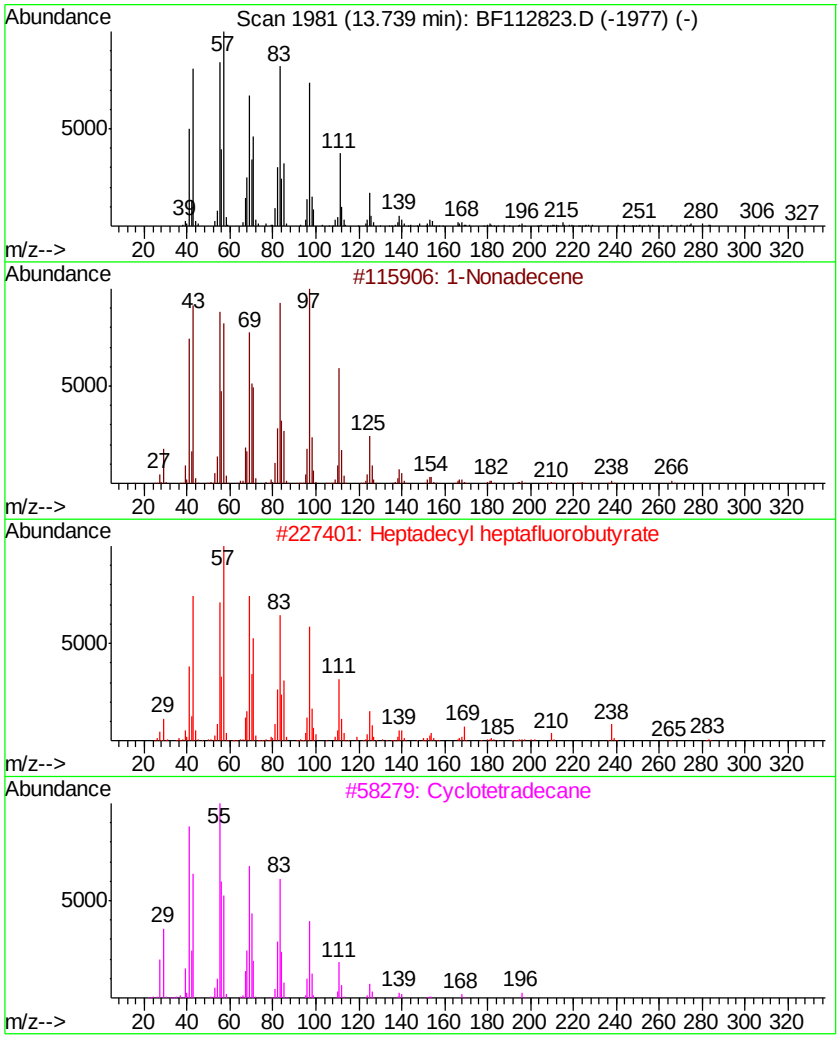
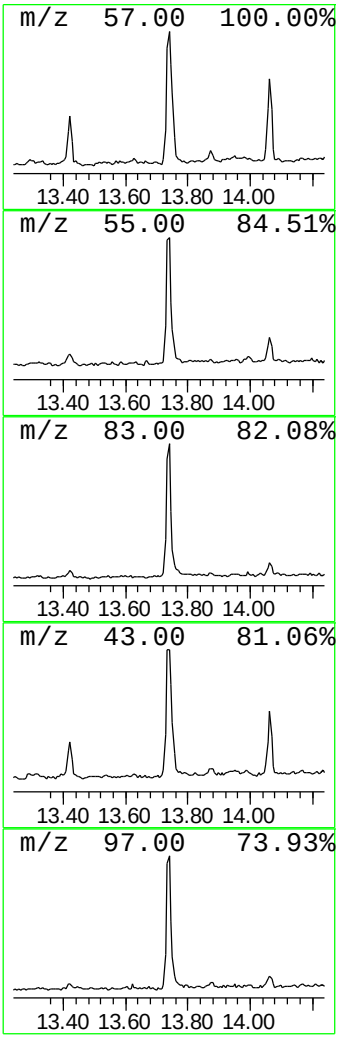
Peak Number 7 1-Nonadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	8.29 ng	577870	Chrysene-d12	13.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	95
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	Cyclotetradecane	196	C14H28	000295-17-0	93
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	93





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Sample : K1707-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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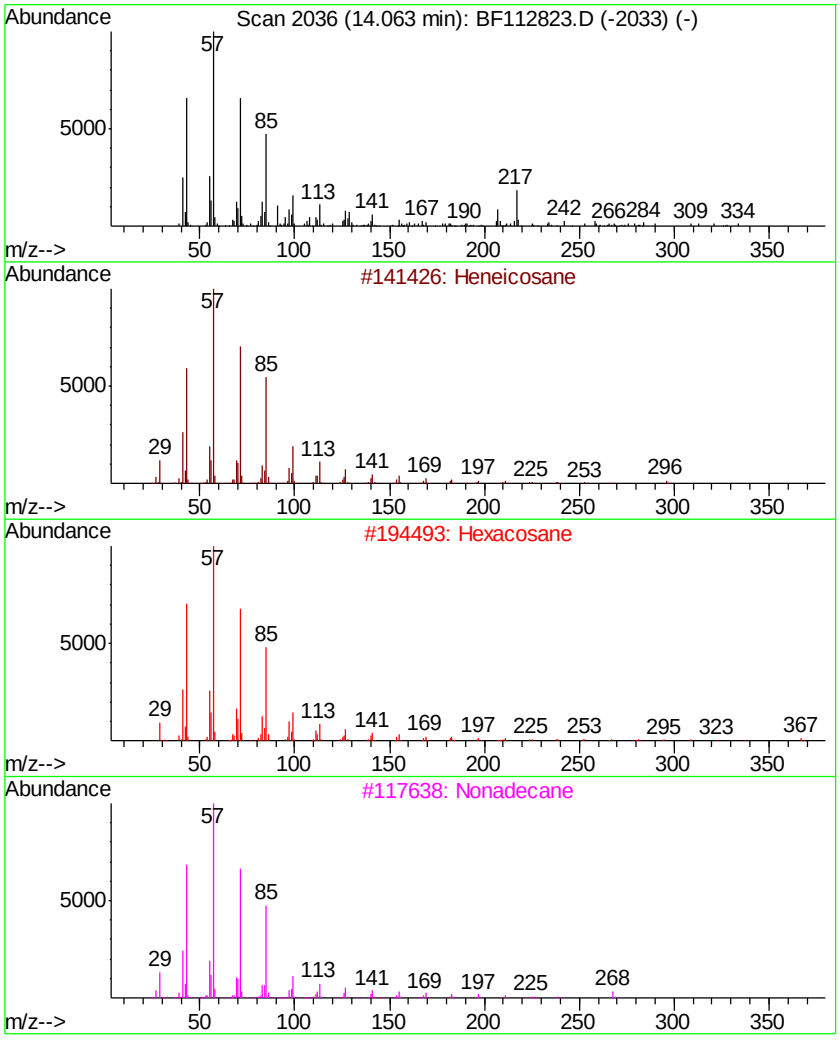
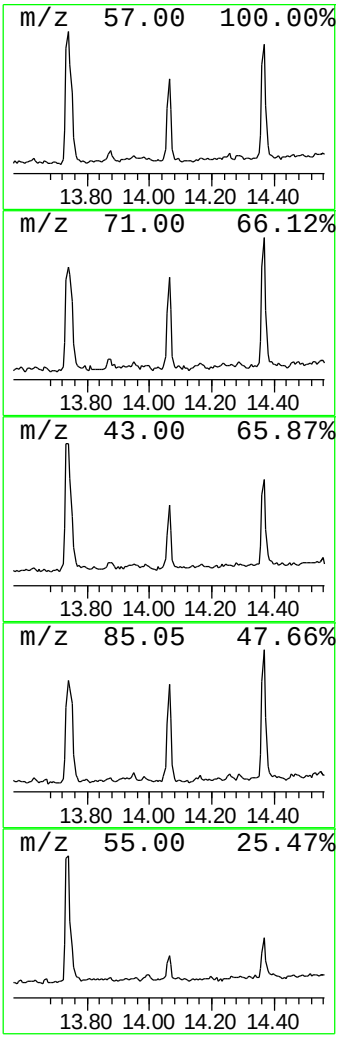
Peak Number 8 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.06	2.29 ng	159624	Chrysene-d12	13.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	87
2	Hexacosane	366	C26H54	000630-01-3	87
3	Nonadecane	268	C19H40	000629-92-5	87
4	Octacosane	394	C28H58	000630-02-4	83
5	Heptadecane	240	C17H36	000629-78-7	83





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Acq On : 4 Mar 2019 14:45
Operator : JU/SJ
Sample : K1707-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12

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

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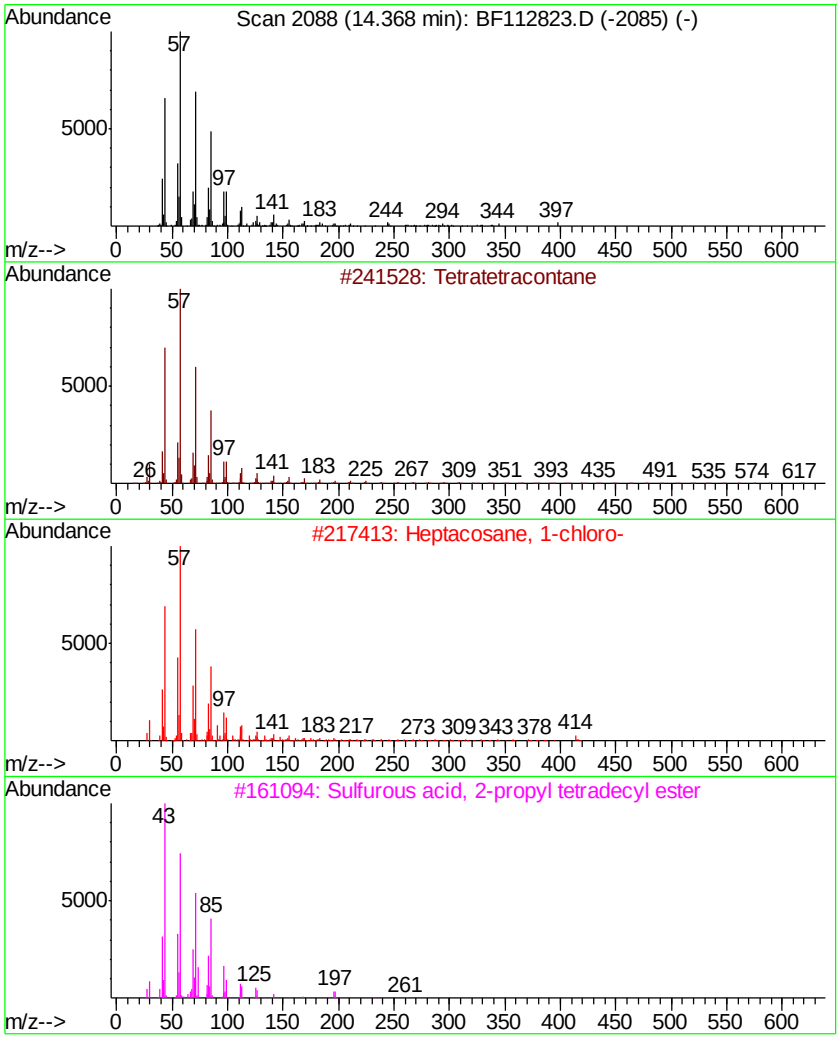
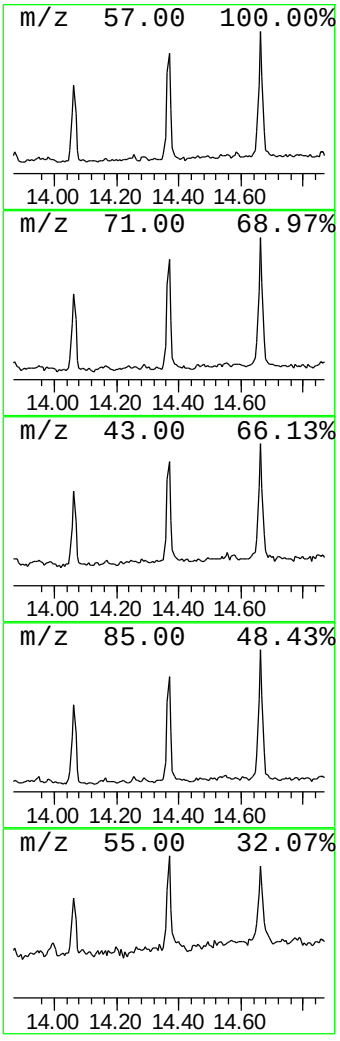
Peak Number 9 Tetratetracontane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.37	2.19 ng	152737	Chrysene-d12	13.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	91
2	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	91
3	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	91
4	2-methyltetracosane	352	C25H52	1000376-72-6	91
5	Hexacosane	366	C26H54	000630-01-3	83





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Sample : K1707-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12

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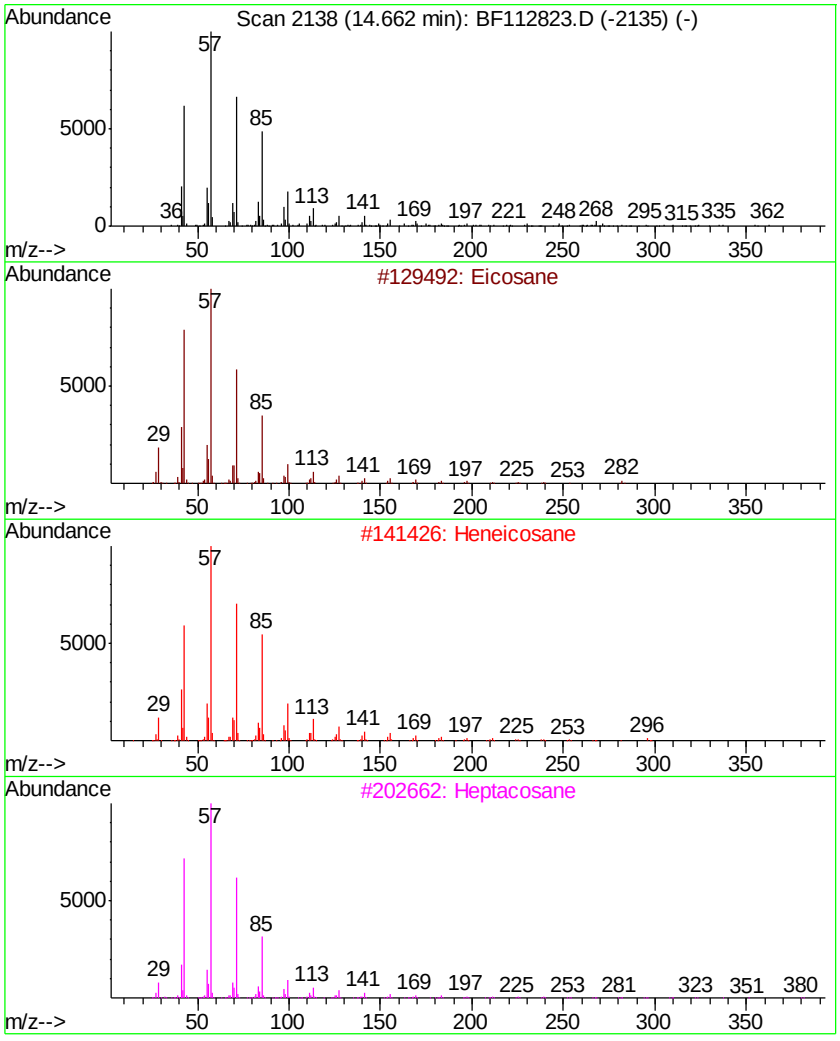
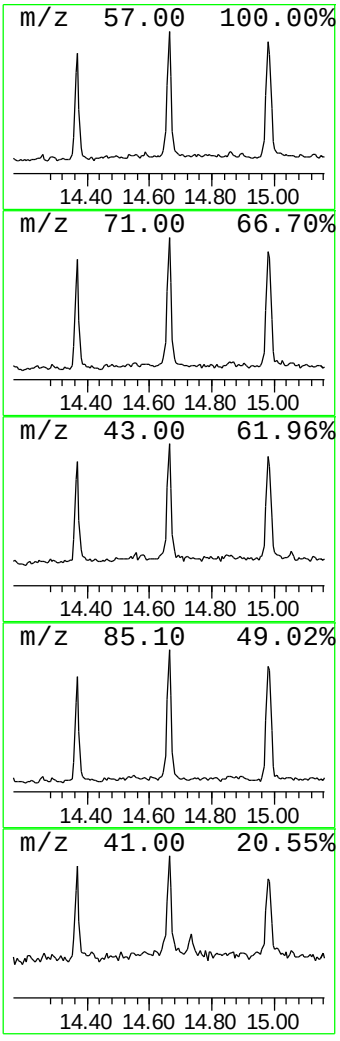
Peak Number 10 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	5.10 ng	269273	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	87
2	Heneicosane	296	C21H44	000629-94-7	72
3	Heptacosane	380	C27H56	000593-49-7	68
4	Hentriacontane	437	C31H64	000630-04-6	64
5	Hexatriacontane	507	C36H74	000630-06-8	64





Library Search Compound Report

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Data File : BF112823.D
Acq On : 4 Mar 2019 14:45
Operator : JU/SJ
Sample : K1707-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
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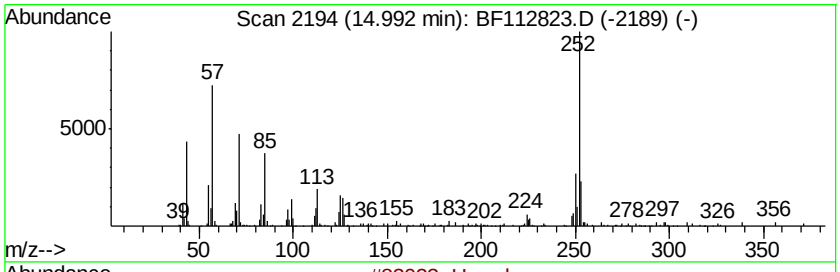
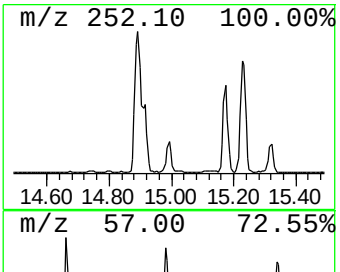
Peak Number 11 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	5.95 ng	313998	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	Heneicosane	296	C21H44	000629-94-7	55
3	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	55
4	Benzo[a]pyrene	252	C20H12	000050-32-8	52
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	50





Library Search Compound Report

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Operator : JU/SJ
Sample : K1707-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12

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TIC Integration Parameters: LSCINT.P

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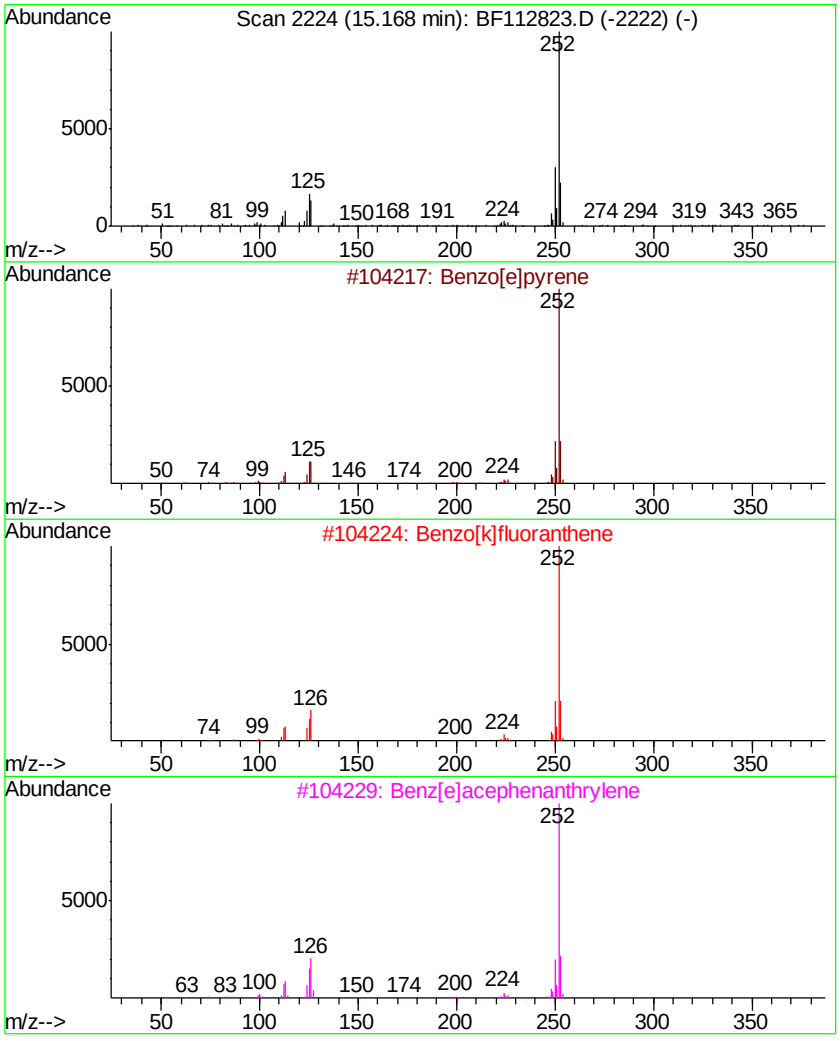
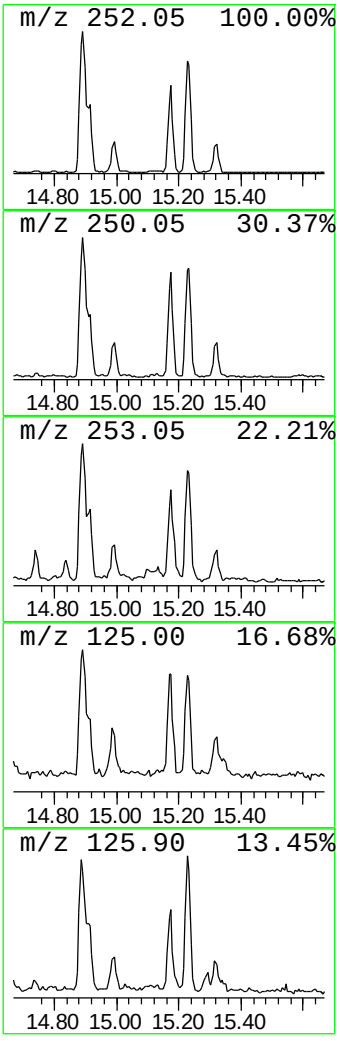
Peak Number 12 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	3.20 ng	168878	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
4	Perylene	252	C20H12	000198-55-0	94
5	Benzo[a]pyrene	252	C20H12	000050-32-8	93





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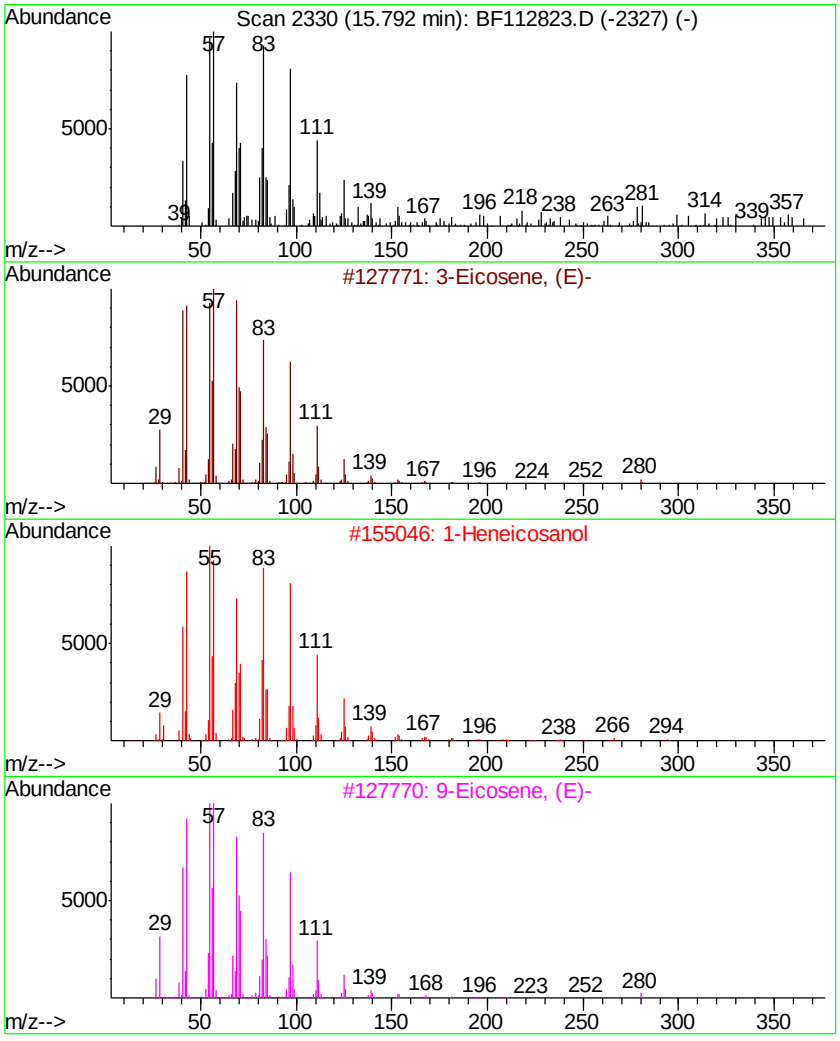
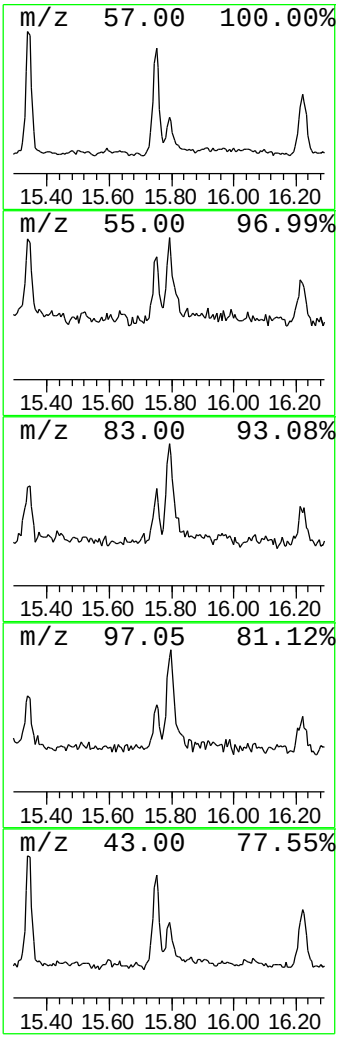
Peak Number 14 3-Eicosene, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	3.91 ng	206553	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	93
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	90





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
unknown6.52	6.52	78.0	ng	3703520	1	6.75	950067	20.0
3-Methyl-4-(metho...	10.69	2.2	ng	127063	4	11.25	1169570	20.0
n-Hexadecanoic acid	11.79	11.1	ng	651521	4	11.25	1169570	20.0
Phenanthrene, 4-m...	11.86	2.6	ng	151019	4	11.25	1169570	20.0
Octadecanoic acid	12.57	3.1	ng	219334	5	13.88	1393750	20.0
1-Nonadecene	13.74	8.3	ng	577870	5	13.88	1393750	20.0
Heneicosane	14.06	2.3	ng	159624	5	13.88	1393750	20.0
Tetratetracontane	14.37	2.2	ng	152737	5	13.88	1393750	20.0
Eicosane	14.66	5.1	ng	269273	6	15.29	1055790	20.0
Hexadecane	14.99	6.0	ng	313998	6	15.29	1055790	20.0
Benzo[e]pyrene	15.17	3.2	ng	168878	6	15.29	1055790	20.0
3-Eicosene, (E)-	15.79	3.9	ng	206553	6	15.29	1055790	20.0