LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112319\
Data File : BF117970.D
Acq On : 23 Nov 2019 21:25
Operator : JU
Sample : K5671-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-112119

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-BF111319.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	2.175	10	15	32	rVB	638753	851203	28.67%	2.391%
2	5.110	507	514	521	rBV	376322	459442	15.47%	1.291%
3	5.516	578	583	586	rBV	2406929	2169527	73.07%	6.095%
4	6.522	749	754	757	rBV	2215140	2294100	77.27%	6.445%
5	6.669	775	779	782	rBV	2733724	2440371	82.20%	6.856%
6	6.904	815	819	822	rBV	887021	723925	24.38%	2.034%
7	7.057	842	845	849	rBV	2030553	1885078	63.49%	5.296%
8	7.463	909	914	917	rBV	1671107	1483322	49.96%	4.167%
9	8.192	1034	1038	1041	rBV	1116294	1052865	35.46%	2.958%
10	9.269	1217	1221	1224	rBV	3592648	2968968	100.00%	8.341%
11	9.663	1285	1288	1296	rVB	451371	398789	13.43%	1.120%
12	9.810	1310	1313	1317	rBV	61375	53098	1.79%	0.149%
13	9.951	1333	1337	1341	rBV	1456985	1253721	42.23%	3.522%
14	9.986	1341	1343	1347	rVB	108787	87808	2.96%	0.247%
15	10.157	1367	1372	1376	rBV	47642	44602	1.50%	0.125%
16	10.504	1427	1431	1437	rVB	85418	85961	2.90%	0.241%
17	10.745	1467	1472	1486	rBV	2117091	2044848	68.87%	5.745%
18	11.245	1554	1557	1562	rVB	36807	34603	1.17%	0.097%
19	11.339	1571	1573	1578	rVB	46374	37239	1.25%	0.105%
20	11.445	1587	1591	1593	rBV	1570149	1325409	44.64%	3.723%
21	11.469	1593	1595	1599	rVV	1000782	778770	26.23%	2.188%
22	11.516	1599	1603	1607	rVB	239058	247511	8.34%	0.695%
23	11.674	1624	1630	1633	rBV	47369	53866	1.81%	0.151%
24	11.898	1664	1668	1672	rBV	136196	148502	5.00%	0.417%
25	11.945	1672	1676	1677	rVV	108802	116892	3.94%	0.328%
26	11.968	1677	1680	1687	rVV2	567884	611540	20.60%	1.718%
27	12.021	1687	1689	1692	rVV	55482	55917	1.88%	0.157%
28	12.063	1692	1696	1698	rVV	174064	197508	6.65%	0.555%
29	12.080	1698	1699	1705	rVB	76180	55913	1.88%	0.157%
30	12.245	1724	1727	1729	rBV	68177	60119	2.02%	0.169%
31	12.268	1729	1731	1734	rVB2	54802	46878	1.58%	0.132%
32	12.498	1767	1770	1773	rBV	75952	76003	2.56%	0.214%
33	12.533	1773	1776	1778	rBV2	43997	43765	1.47%	0.123%
34	12.586	1782	1785	1790	rVB2	49582	55148	1.86%	0.155%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
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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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Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.663	1794	1798	1801	rBV	1154408	999050	33.65%	2.807%
36	12.751	1811	1813	1817	rBV	161131	158926	5.35%	0.446%
37	12.892	1831	1837	1843	rVV	976892	975580	32.86%	2.741%
38	12.939	1843	1845	1850	rVB2	47598	55633	1.87%	0.156%
39	13.033	1857	1861	1865	rVB	2765473	2388834	80.46%	6.711%
40	13.110	1869	1874	1878	rBV3	61137	110425	3.72%	0.310%
41	13.198	1885	1889	1890	rBV3	51963	54662	1.84%	0.154%
42	13.221	1890	1893	1896	rVB	127867	116331	3.92%	0.327%
43	13.286	1901	1904	1907	rVB2	103238	77709	2.62%	0.218%
44	13.321	1907	1910	1913	rBV2	84370	88990	3.00%	0.250%
45	13.415	1923	1926	1929	rBV	52132	44404	1.50%	0.125%
46	13.445	1929	1931	1935	rVV	43584	46890	1.58%	0.132%
47	13.604	1954	1958	1960	rBV3	29926	38468	1.30%	0.108%
48	13.727	1976	1979	1983	rVB	58143	64525	2.17%	0.181%
49	13.839	1993	1998	2001	rBV2	75443	112931	3.80%	0.317%
50	13.868	2001	2003	2005	rVV	83405	74103	2.50%	0.208%
51	13.892	2005	2007	2011	rVV2	79052	116877	3.94%	0.328%
52	13.933	2011	2014	2026	rVB3	225198	349697	11.78%	0.982%
53	14.092	2034	2041	2044	rBV2	1054974	1341362	45.18%	3.768%
54	14.115	2044	2045	2051	rVB	383901	311234	10.48%	0.874%
55	14.198	2057	2059	2062	rVB	68785	53634	1.81%	0.151%
56	14.315	2075	2079	2082	rBV2	35201	49563	1.67%	0.139%
57	14.480	2102	2107	2110	rVB	74323	76229	2.57%	0.214%
58	14.515	2110	2113	2116	rVB2	46672	44885	1.51%	0.126%
59	14.562	2117	2121	2125	rBV4	67295	119785	4.03%	0.337%
60	14.604	2126	2128	2130	rVV	57308	51468	1.73%	0.145%
61	14.627	2130	2132	2135	rVB2	57071	49512	1.67%	0.139%
62	14.874	2171	2174	2177	rBV	62891	58431	1.97%	0.164%
63	14.957	2184	2188	2191	rBV	95534	109616	3.69%	0.308%
64	15.151	2216	2221	2224	rBV	359329	544003	18.32%	1.528%
65	15.227	2231	2234	2237	rVV2	60450	62673	2.11%	0.176%
66	15.262	2237	2240	2245	rVB	77558	90730	3.06%	0.255%
67	15.468	2271	2275	2281	rVB	211218	263349	8.87%	0.740%
68	15.533	2281	2286	2292	rBV	307360	401993	13.54%	1.129%
69	15.598	2292	2297	2300	rVV	673263	847377	28.54%	2.381%
70	15.627	2300	2302	2310	rVB2	151801	190557	6.42%	0.535%
71	16.086	2377	2380	2386	rVB3	43188	56465	1.90%	0.159%

LSC Area Percent Report

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Instrument : BNA_F
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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	16.615	2466	2470	2475	rBV4	29453	49497	1.67%	0.139%
73	17.115	2550	2555	2566	rVB2	159139	331783	11.18%	0.932%
74	17.574	2627	2633	2645	rBV	122993	278385	9.38%	0.782%
75	17.686	2646	2652	2657	rBV5	43028	96153	3.24%	0.270%

Sum of corrected areas: 35595930

LSC Report - Integrated Chromatogram

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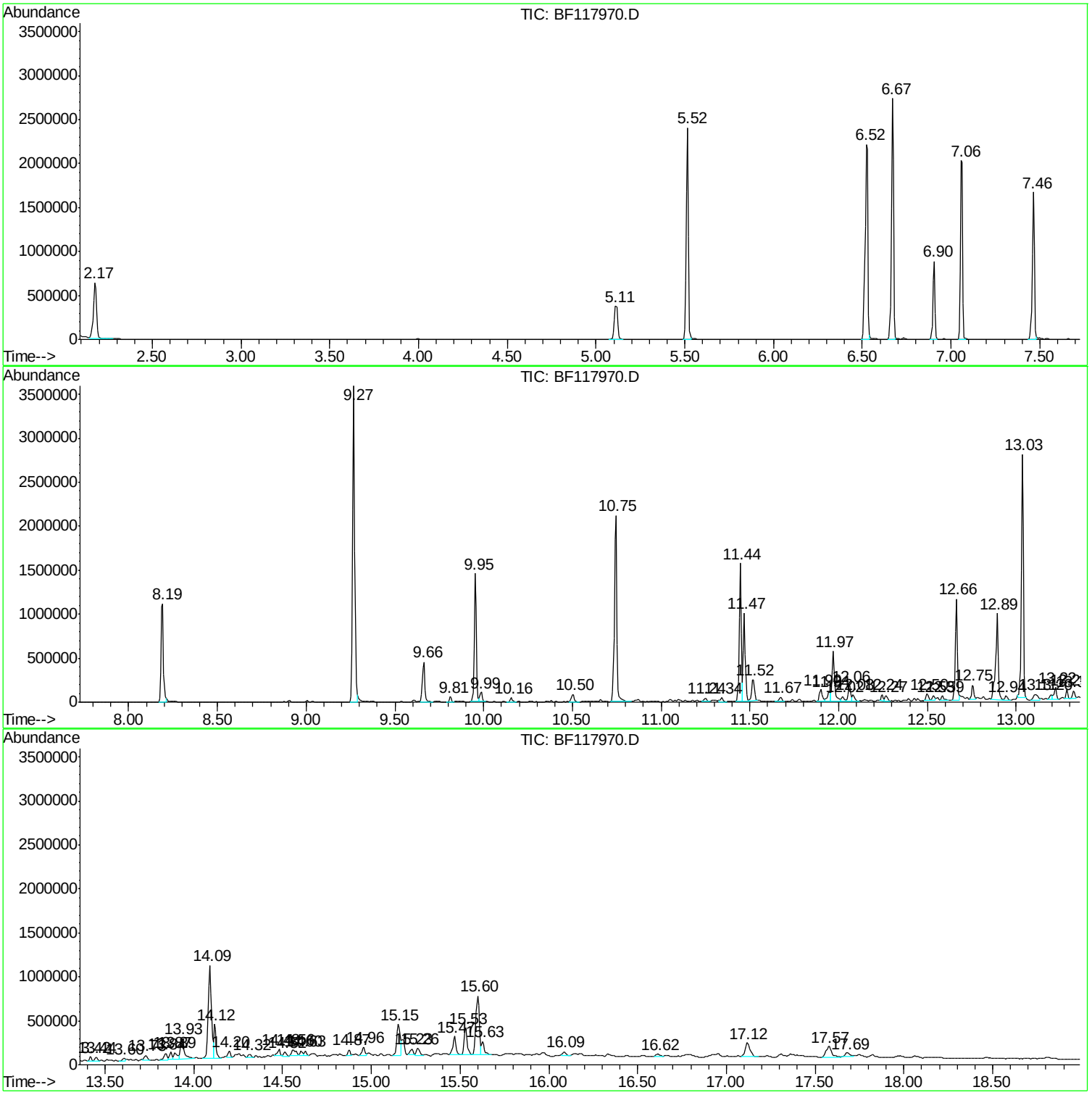
Acq On : 23 Nov 2019 21:25
Operator : JU
Sample : K5671-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-112119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112319\
Data File : BF117970.D
Acq On : 23 Nov 2019 21:25
Operator : JU
Sample : K5671-11
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Instrument : BNA_F
ClientSampleId : OR-02-112119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

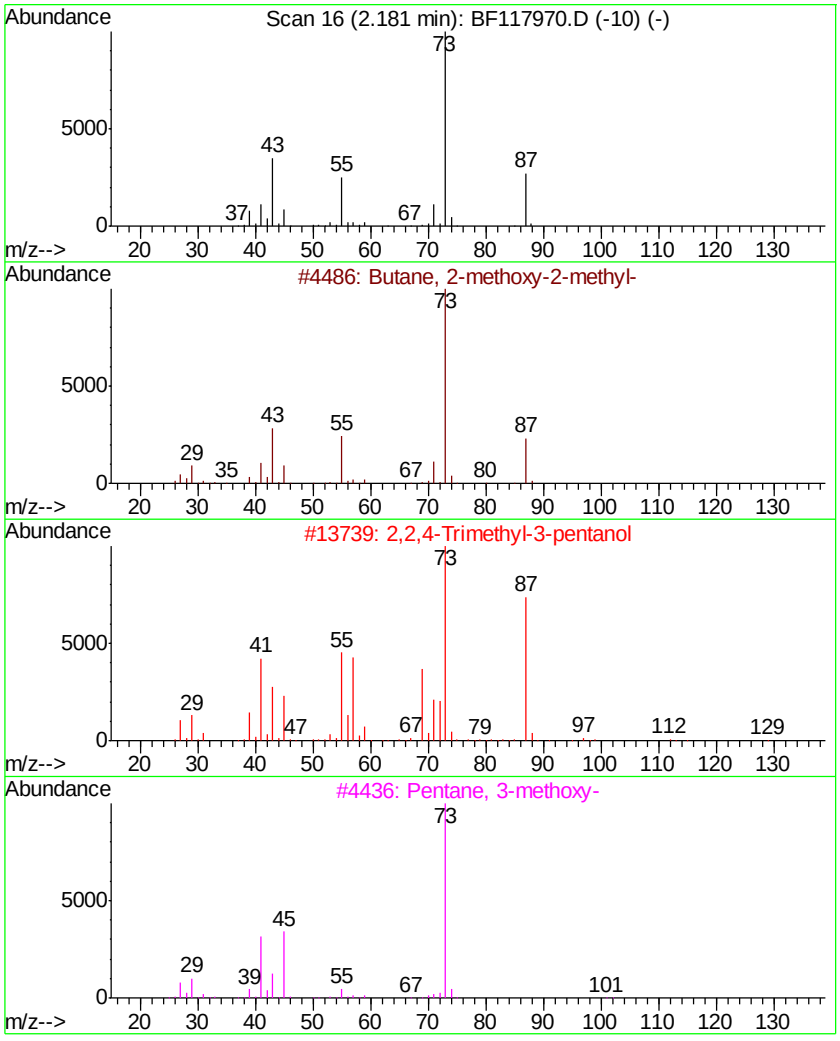
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

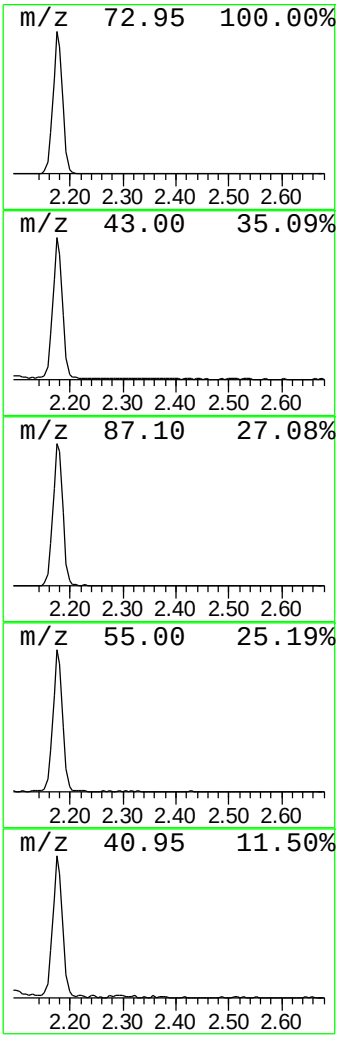
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	23.52 ng	851203	1,4-Dichlorobenzene-d4	6.90

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	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





Library Search Compound Report

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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-112119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

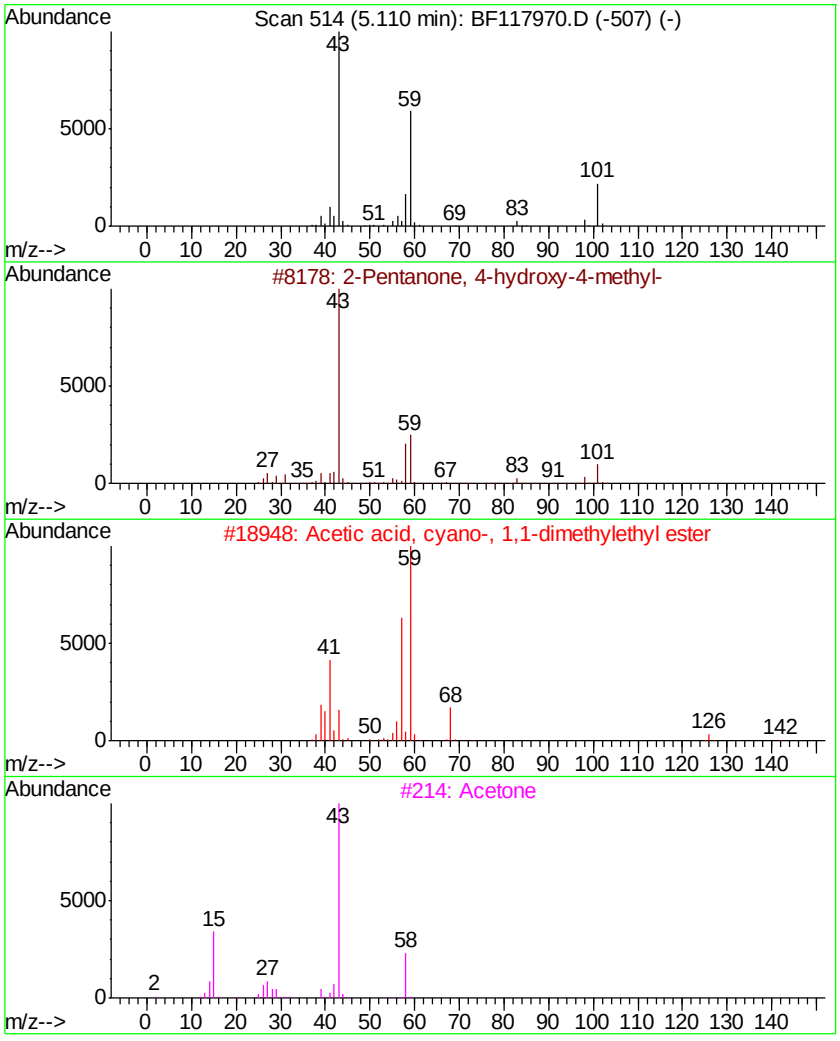
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

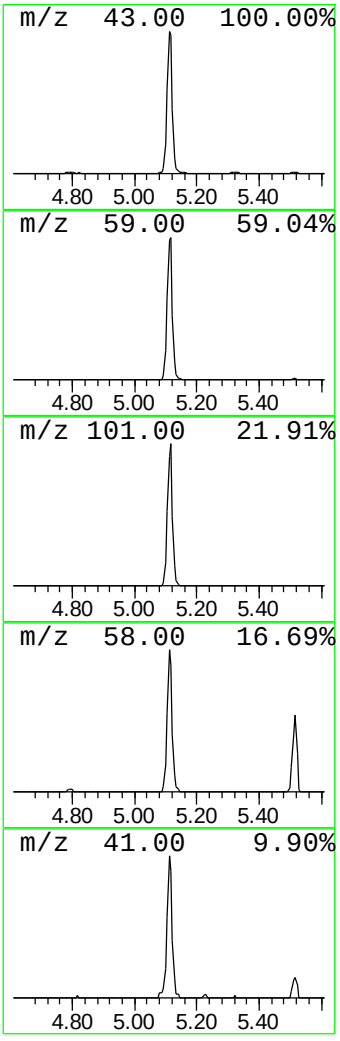
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	12.69 ng	459442	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Acetone	58	C3H6O	000067-64-1	10
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112319\
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Instrument : BNA_F
ClientSampleId : OR-02-112119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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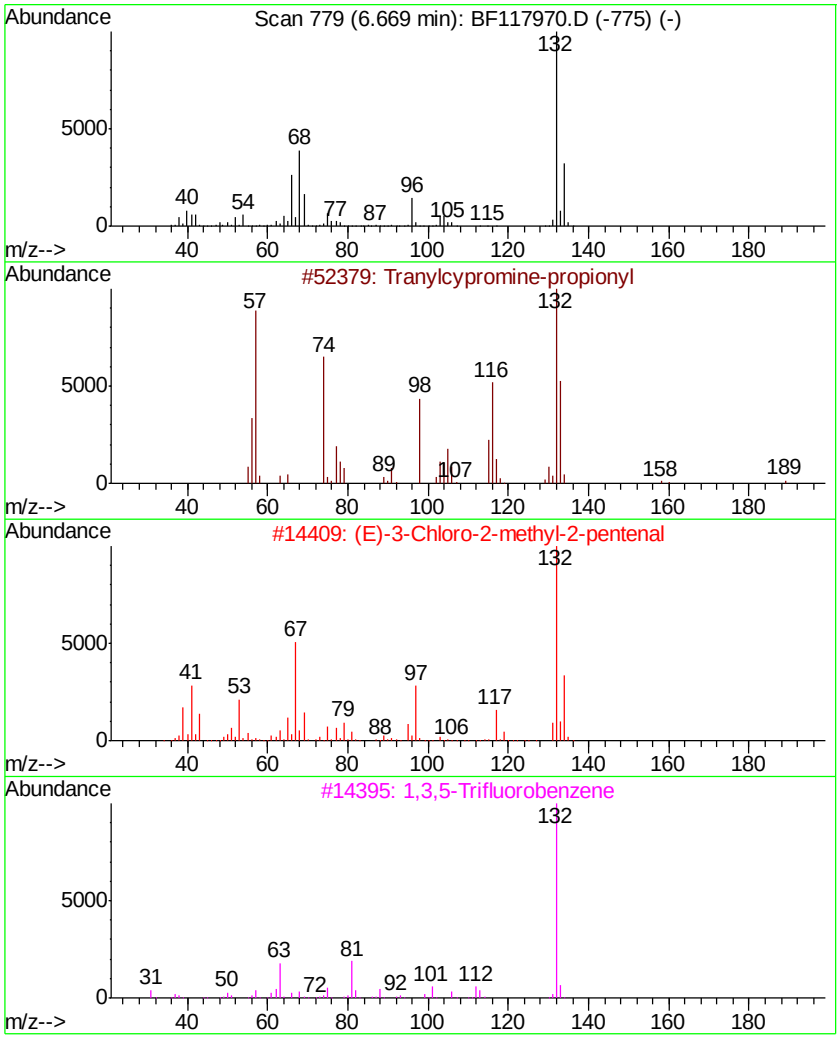
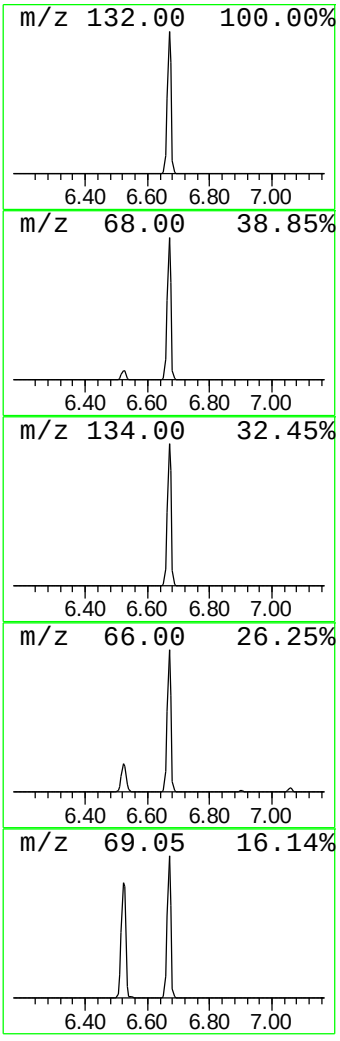
****

Peak Number 3 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	67.42 ng	2440370	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	Xenon	132	Xe	007440-63-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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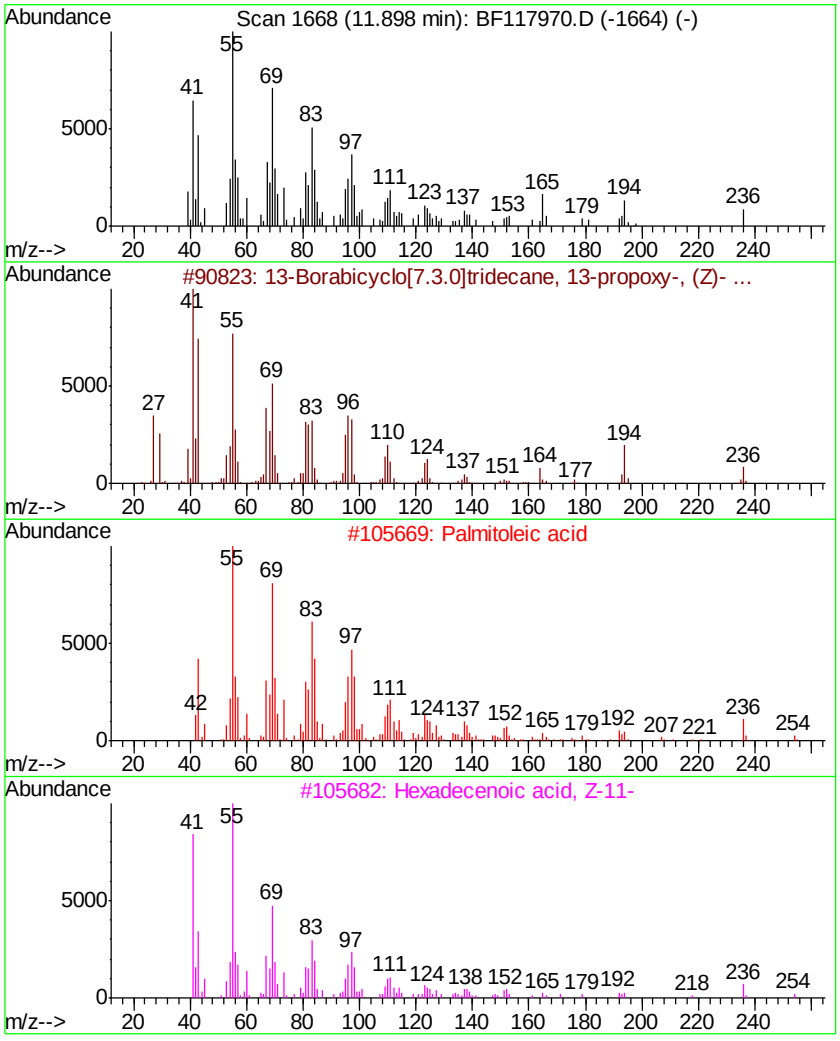
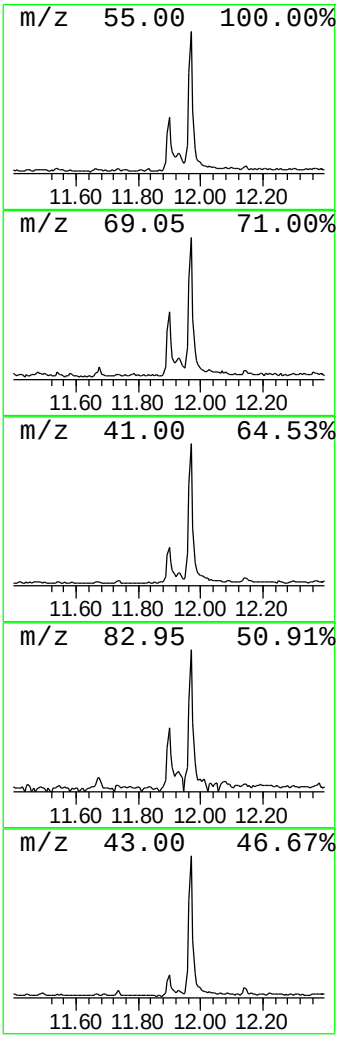
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 13-Borabicyclo[7.3.0]tridec... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	2.24 ng	148502	Phenanthrene-d10	11.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Borabicyclo[7.3.0]tridecane, ...	236	C15H29BO	1000156-41-7	95
2	Palmitoleic acid	254	C16H30O2	000373-49-9	94
3	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	90
4	cis-9-Hexadecenoic acid	254	C16H30O2	1000333-19-5	87
5	1,9-Tetradecadiene	194	C14H26	112929-06-3	72





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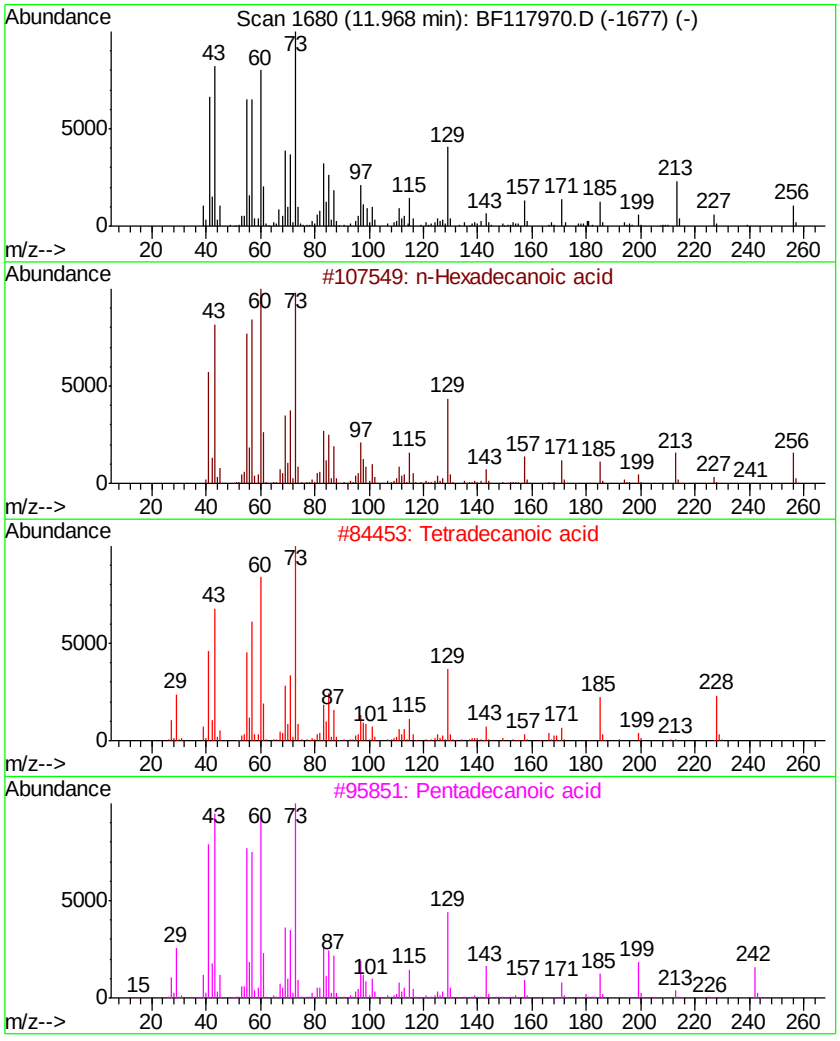
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

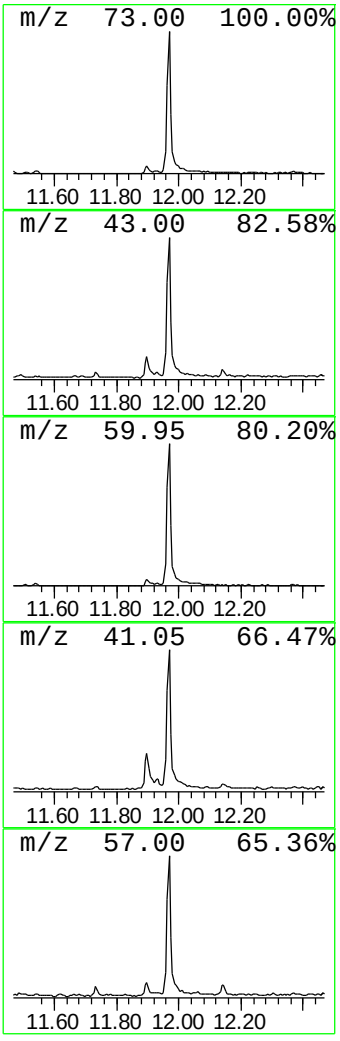
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.97	9.23 ng	611540	Phenanthrene-d10	11.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tridecanoic acid	214	C13H26O2	000638-53-9	90
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-112119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

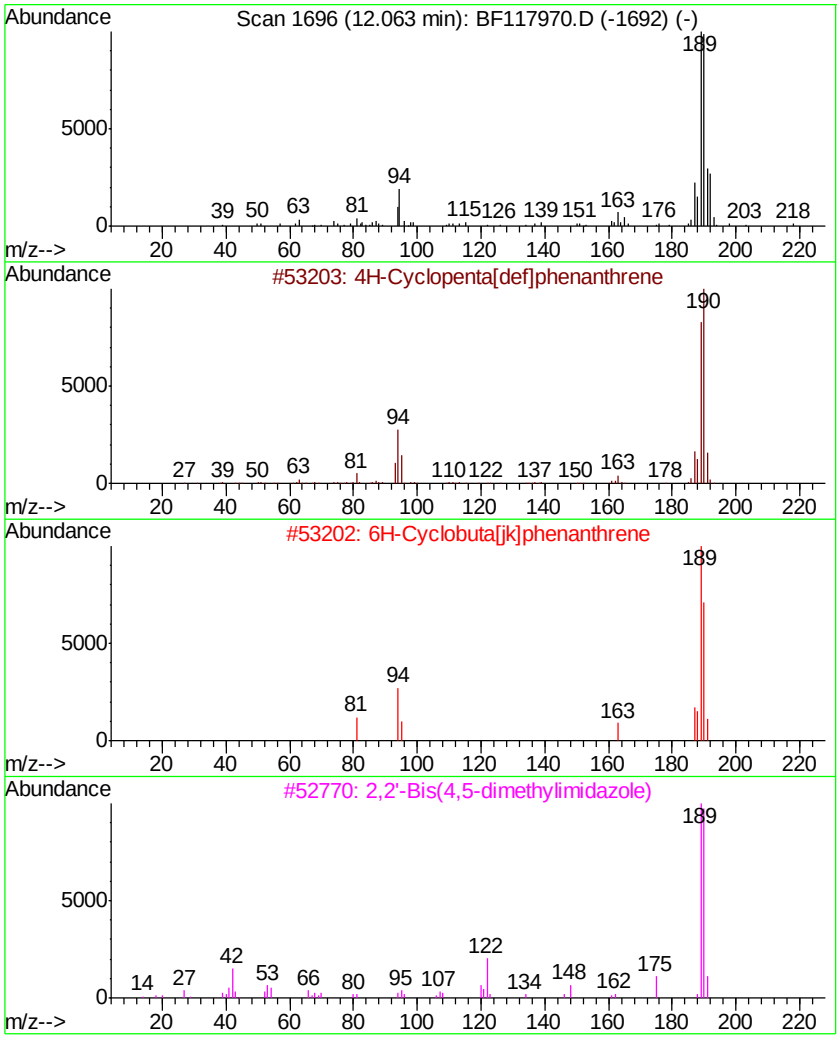
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

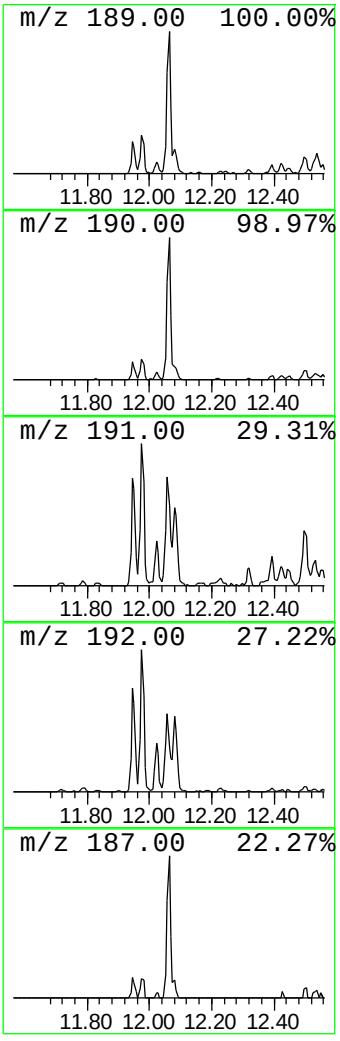
****

Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.06	2.98 ng	197508	Phenanthrene-d10	11.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	72
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
4	Pyrimidine, 2-chloro-5-phenyl-	190	C10H7ClN2	022536-62-5	25
5	1-Aminocyclopentanecarboxylic ac...	431	C23H42ClNO4	1000329-17-4	16





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Data File : BF117970.D
Acq On : 23 Nov 2019 21:25
Operator : JU
Sample : K5671-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-112119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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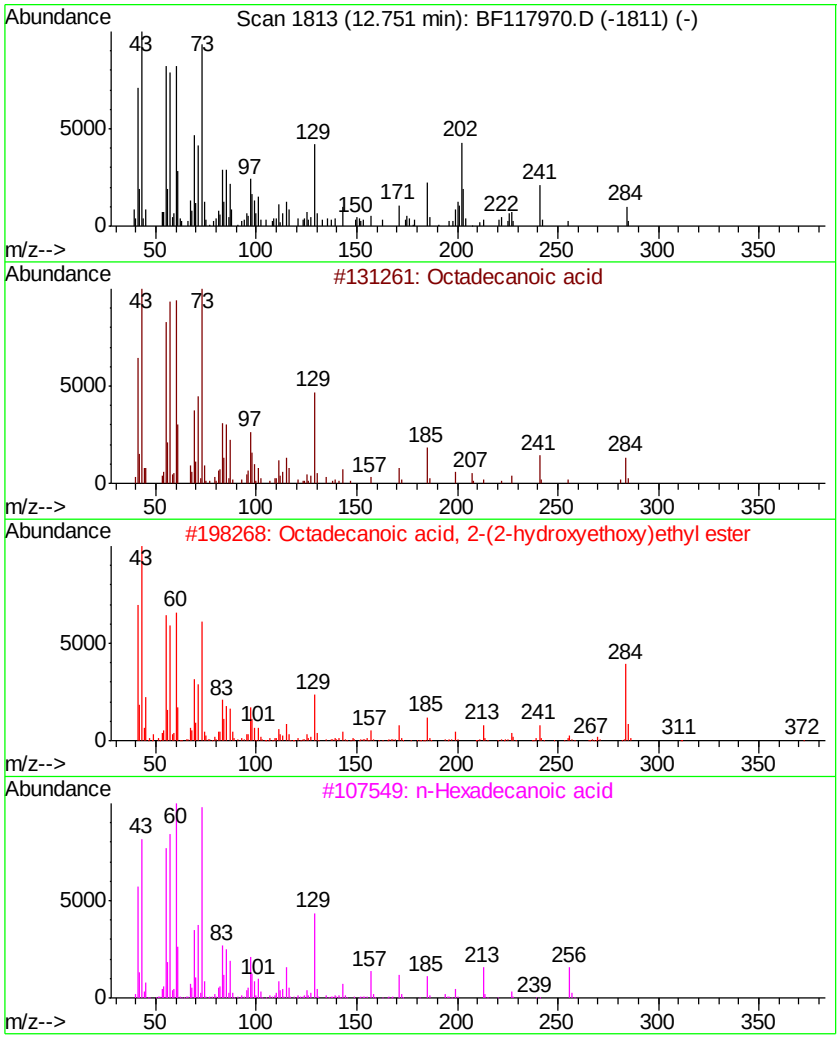
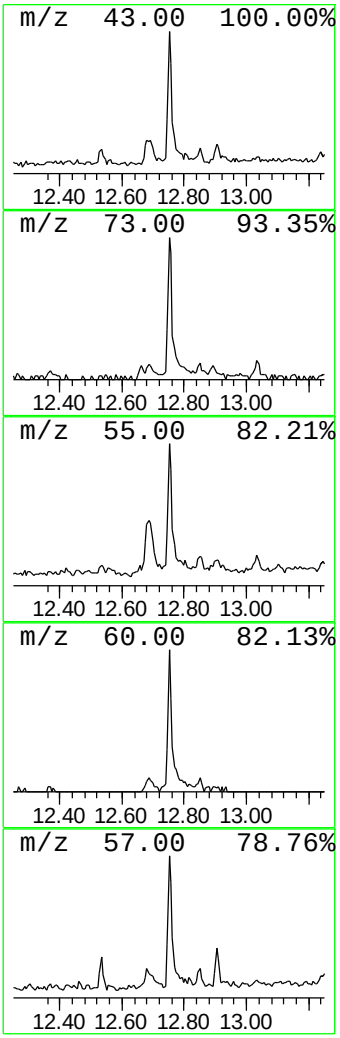
Peak Number 8 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.75	2.40 ng	158926	Phenanthrene-d10	11.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	74
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	62





Library Search Compound Report

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Data File : BF117970.D
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Operator : JU
Sample : K5671-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-112119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
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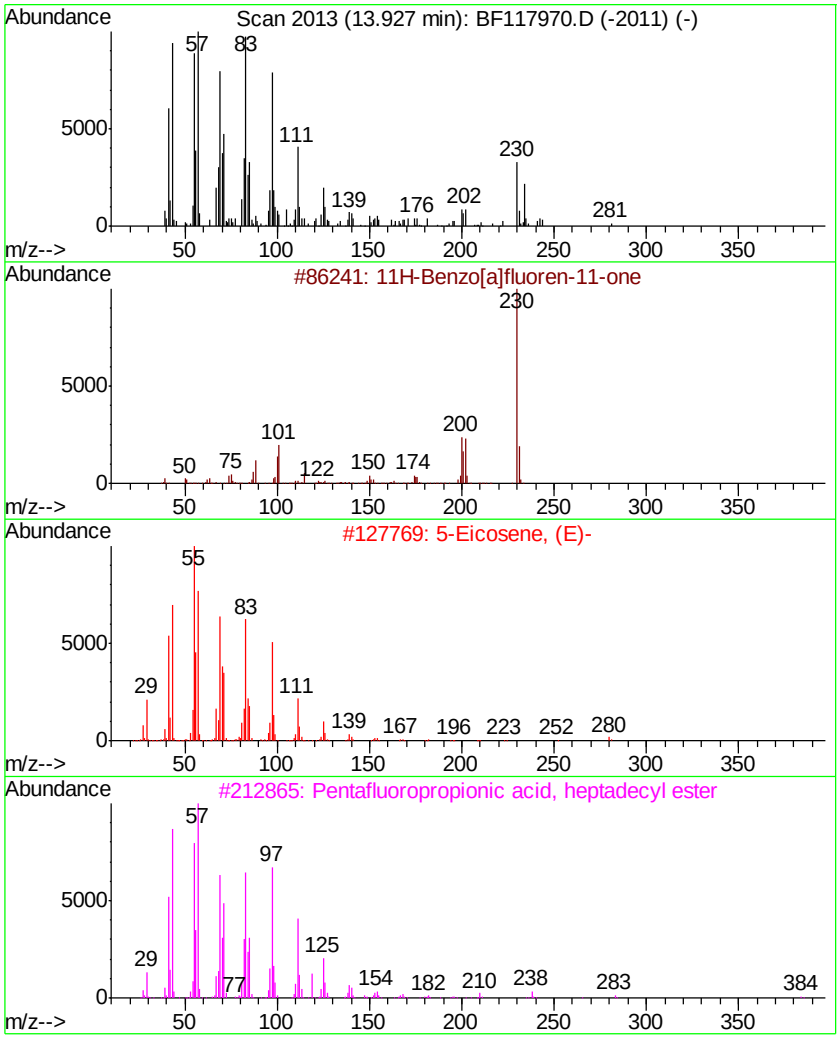
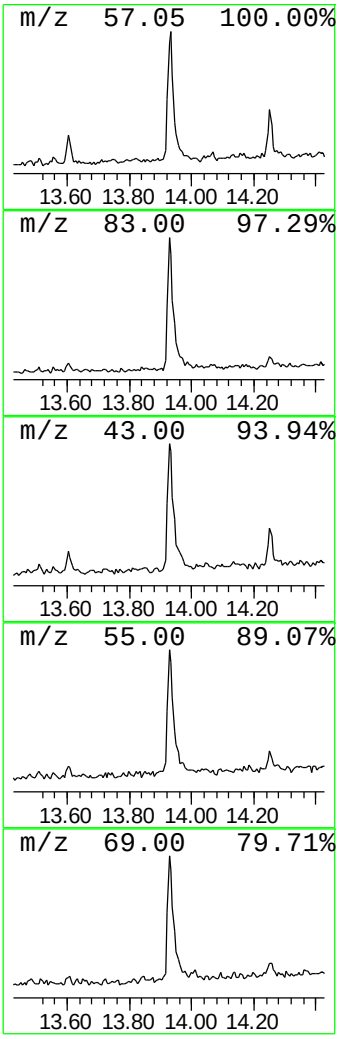
Peak Number 9 11H-Benzo[a]fluoren-11-one Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	5.21 ng	349697	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	93
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	84
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	70
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	55
5	Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	55





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Data File : BF117970.D
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Operator : JU
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ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-112119

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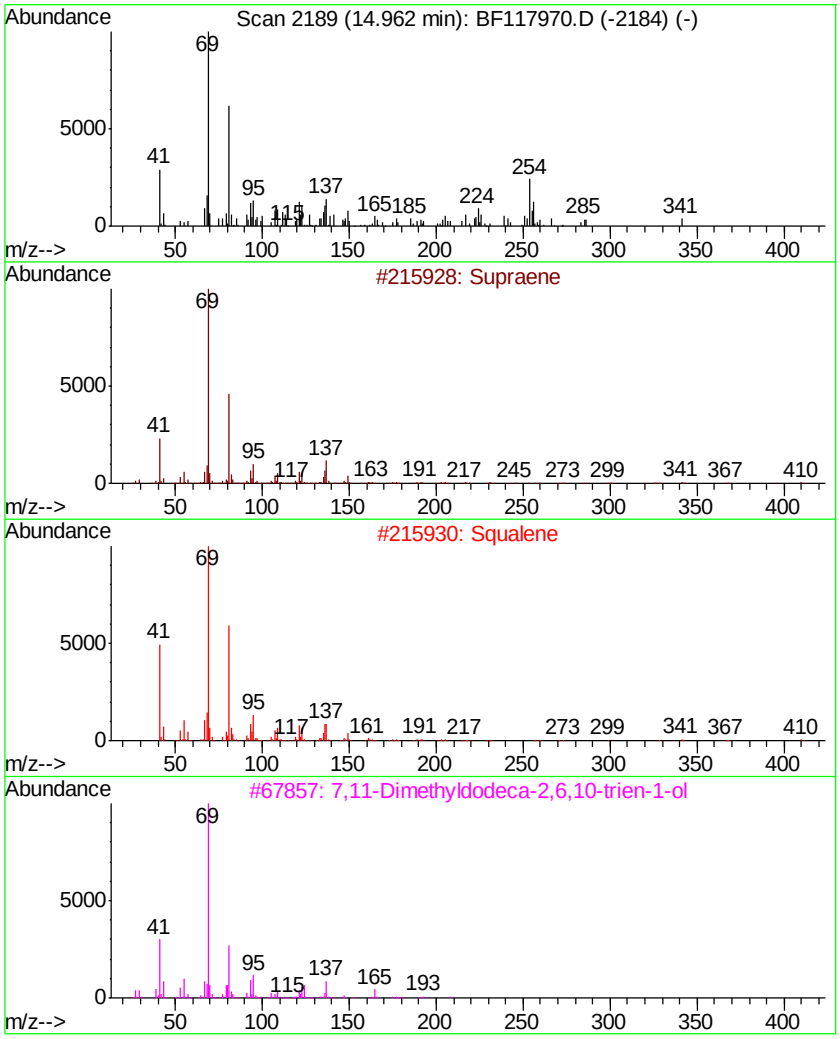
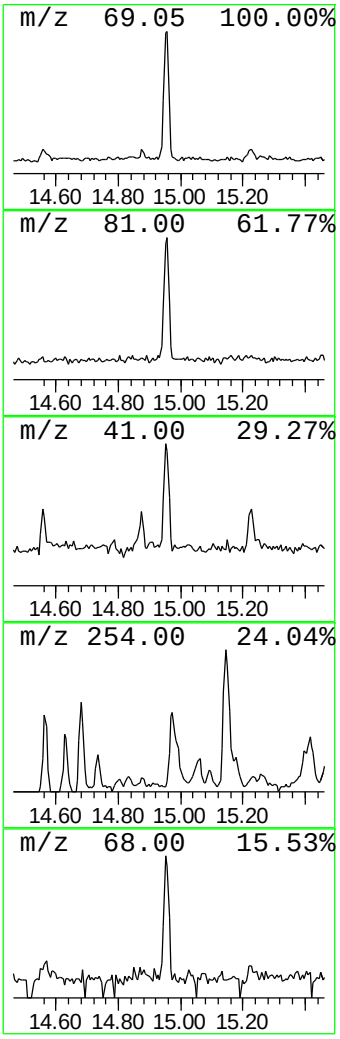
Peak Number 10 Supraene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	2.59 ng	109616	Perylene-d12	15.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	81
2	Squalene	410	C30H50	000111-02-4	81
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	68
5	2,6,10-Dodecatrienoic acid, 3,7,...	250	C16H26O2	003675-00-1	64





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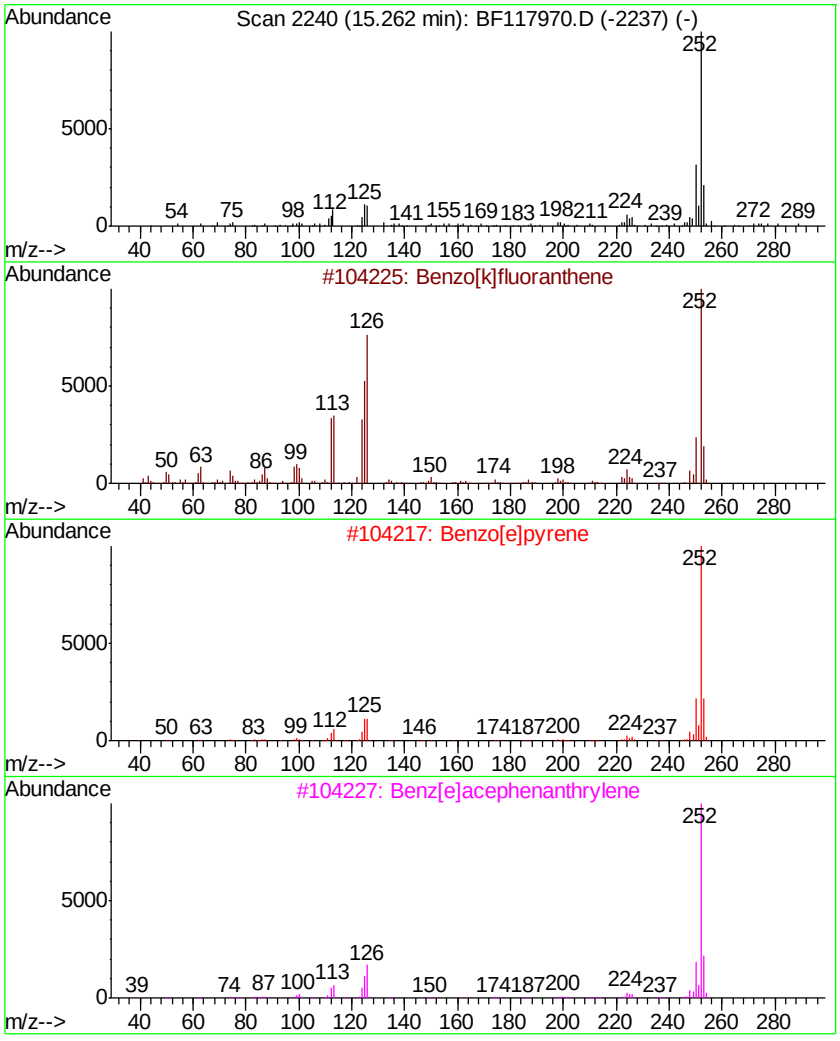
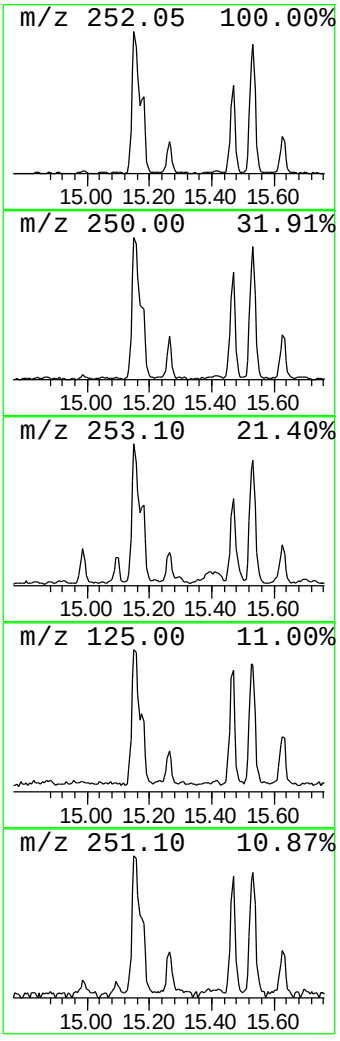
Peak Number 11 Benzo[e]pyrene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.26	2.14 ng	90730	Perylene-d12	15.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
2	Benzo[e]pyrene	252	C20H12	000192-97-2	93
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	90
4	Benzo[a]pyrene	252	C20H12	000050-32-8	81
5	Perylene	252	C20H12	000198-55-0	81





Library Search Compound Report

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ClientSampleId : OR-02-112119

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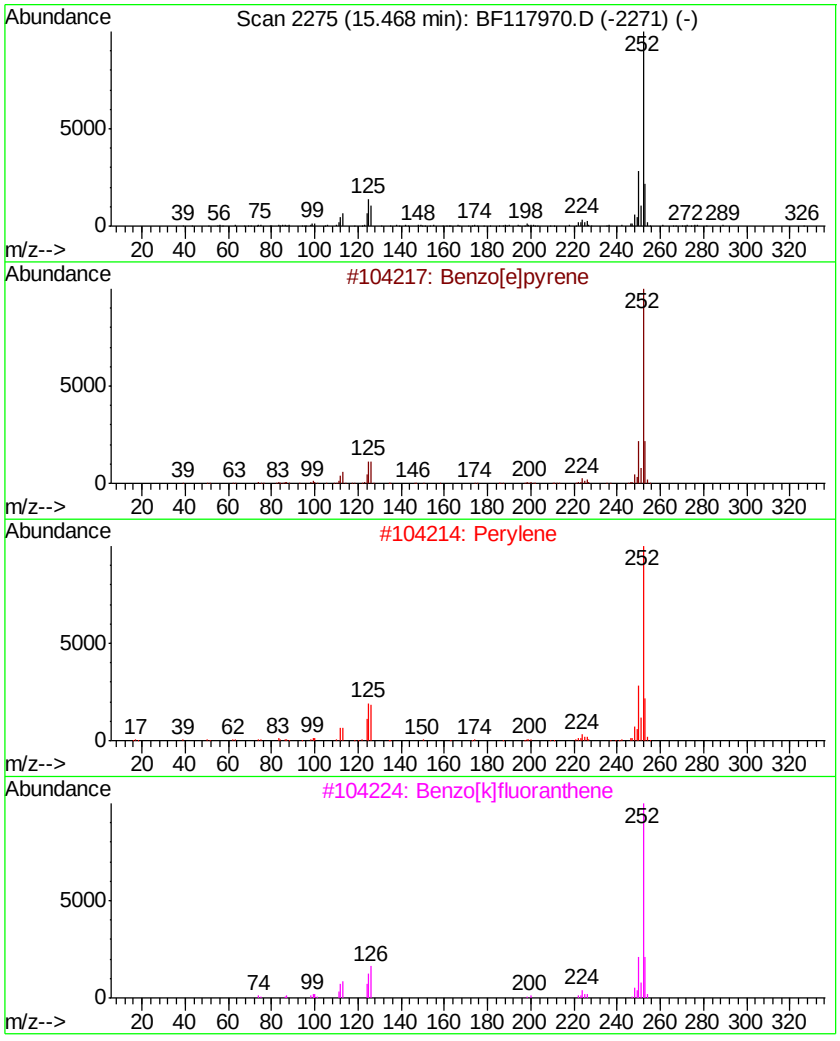
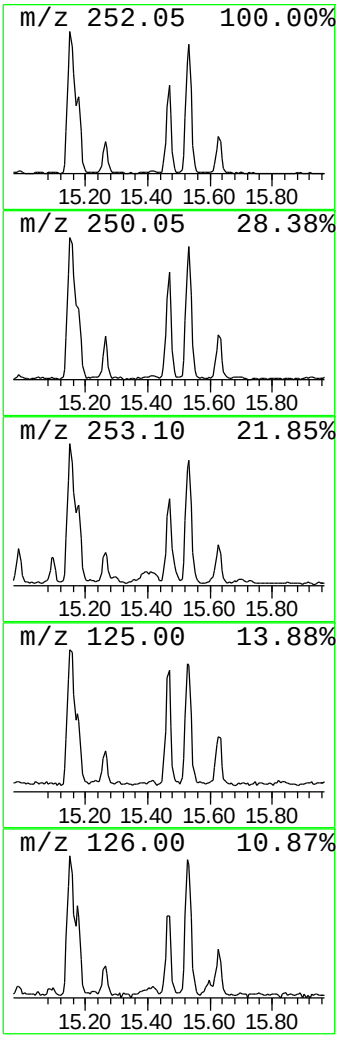
Peak Number 12 Perylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.47	6.22 ng	263349	Perylene-d12	15.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Perylene	252	C20H12	000198-55-0	97
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
4	Benzo[a]pyrene	252	C20H12	000050-32-8	95
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95





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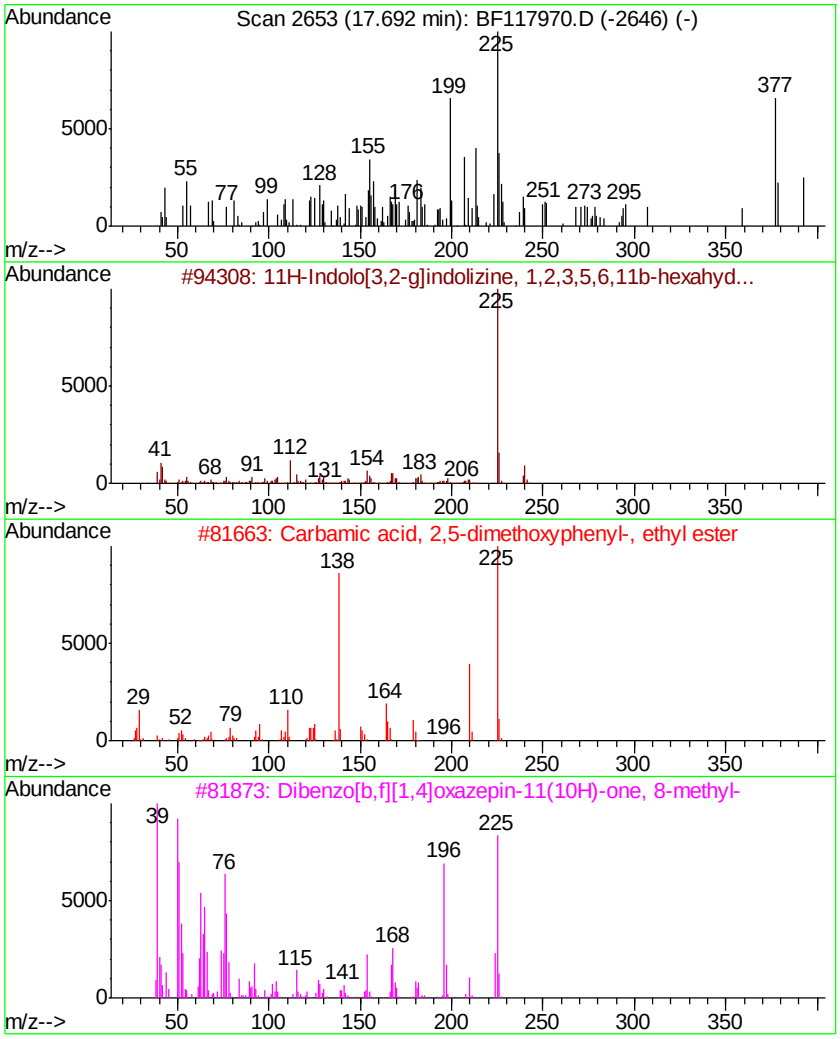
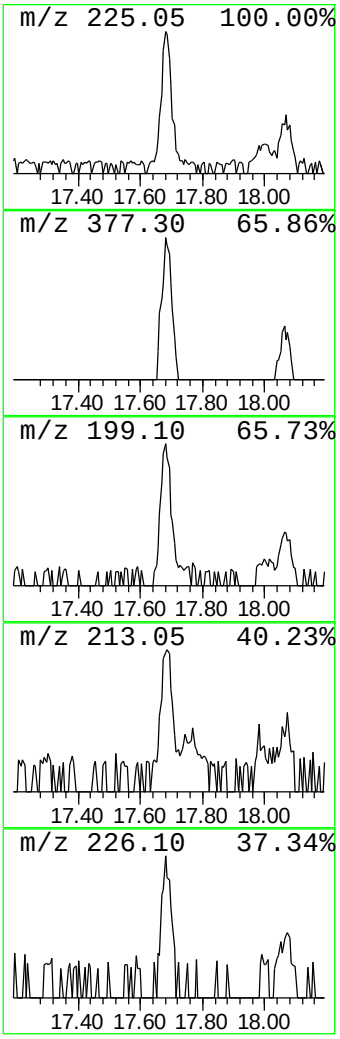
Peak Number 13 unknown17.69 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.69	2.27 ng	96153	Perylene-d12	15.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Indolo[3,2-g]indolizine, 1,2...	240	C16H20N2	1000264-72-5	22
2	Carbamic acid, 2,5-dimethoxyphen...	225	C11H15NO4	1000314-76-1	20
3	Dibenzo[b,f][1,4]oxazepin-11(10H...	225	C14H11NO2	1000362-72-5	18
4	(3-Isopropyl-5-methylamino-2,4,6...	225	C14H15N3	014204-00-3	18
5	4-Thiazolemethanol, 2-(4-chlorop...	225	C10H8ClNOS	036093-99-9	18





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.18	23.5	ng	851203	1	6.90	723925	20.0
2-Pentanone, 4-hy...	5.11	12.7	ng	459442	1	6.90	723925	20.0
unknown6.67	6.67	67.4	ng	2440370	1	6.90	723925	20.0
13-Borabicyclo[7....	11.90	2.2	ng	148502	4	11.45	1325410	20.0
n-Hexadecanoic acid	11.97	9.2	ng	611540	4	11.45	1325410	20.0
4H-Cyclopenta[def...	12.06	3.0	ng	197508	4	11.45	1325410	20.0
Octadecanoic acid	12.75	2.4	ng	158926	4	11.45	1325410	20.0
11H-Benzo[a]fluor...	13.93	5.2	ng	349697	5	14.09	1341360	20.0
Supraene	14.96	2.6	ng	109616	6	15.60	847377	20.0
Benzo[e]pyrene	15.26	2.1	ng	90730	6	15.60	847377	20.0
Perylene	15.47	6.2	ng	263349	6	15.60	847377	20.0
unknown17.69	17.69	2.3	ng	96153	6	15.60	847377	20.0