LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110819\
Data File : BF117744.D
Acq On : 8 Nov 2019 21:10
Operator : JU
Sample : K5722-20
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3-D

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-BF110619.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	2.240	20	26	43	rVB	1540268	2168285	26.49%	2.065%
2	5.151	515	521	530	rVB	1393958	1727188	21.10%	1.645%
3	5.545	582	588	591	rBV	6723080	6878145	84.02%	6.551%
4	6.551	752	759	762	rBV	6577598	7433307	90.80%	7.079%
5	6.698	779	784	787	rBV	7489466	7457747	91.10%	7.103%
6	6.928	819	823	827	rBV	2641226	2099698	25.65%	2.000%
7	7.086	846	850	853	rBV	6760411	5818718	71.08%	5.542%
8	7.492	913	919	922	rBV	4581329	4872341	59.52%	4.640%
9	8.216	1037	1042	1045	rBV	3230961	2824212	34.50%	2.690%
10	9.292	1220	1225	1228	rBV	8480787	8186297	100.00%	7.797%
11	9.404	1240	1244	1248	rVB2	137233	153510	1.88%	0.146%
12	9.686	1288	1292	1295	rVB	986658	857675	10.48%	0.817%
13	9.833	1314	1317	1320	rBV	268180	208170	2.54%	0.198%
14	9.975	1337	1341	1345	rBV	3863079	3269561	39.94%	3.114%
15	10.769	1470	1476	1479	rBV	5846620	5846962	71.42%	5.569%
16	10.863	1489	1492	1494	rBV	172944	151564	1.85%	0.144%
17	10.892	1494	1497	1503	rVB5	109362	135573	1.66%	0.129%
18	11.269	1558	1561	1565	rVB	125604	122680	1.50%	0.117%
19	11.327	1565	1571	1575	rBV5	100730	161797	1.98%	0.154%
20	11.469	1591	1595	1597	rBV	4019071	3469885	42.39%	3.305%
21	11.492	1597	1599	1602	rVV	861974	662935	8.10%	0.631%
22	11.539	1602	1607	1610	rVV	385742	392310	4.79%	0.374%
23	11.686	1628	1632	1636	rBV	362468	407445	4.98%	0.388%
24	11.969	1677	1680	1681	rBV	259866	210517	2.57%	0.200%
25	11.992	1681	1684	1688	rVB2	1505092	1344770	16.43%	1.281%
26	12.080	1695	1699	1701	rBV2	327515	340139	4.15%	0.324%
27	12.104	1701	1703	1707	rVB	200365	157939	1.93%	0.150%
28	12.169	1708	1714	1717	rBV3	98709	139879	1.71%	0.133%
29	12.245	1724	1727	1729	rBV	347857	286647	3.50%	0.273%
30	12.286	1732	1734	1739	rVB	263185	200283	2.45%	0.191%
31	12.510	1769	1772	1777	rBV3	759491	874012	10.68%	0.832%
32	12.557	1777	1780	1782	rVV2	167277	167790	2.05%	0.160%
33	12.604	1785	1788	1794	rVB	231539	226989	2.77%	0.216%
34	12.686	1798	1802	1805	rBV	2835730	2601238	31.78%	2.477%

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Misc :
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Instrument : BNA_F
ClientSampleId : 3-D

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
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If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.716	1805	1807	1810	rBV3	101133	84708	1.03%	0.081%
36	12.774	1815	1817	1820	rBV	446439	386460	4.72%	0.368%
37	12.916	1835	1841	1846	rBV	2682227	2866212	35.01%	2.730%
38	12.963	1846	1849	1853	rVB2	138542	192172	2.35%	0.183%
39	13.063	1861	1866	1869	rVB	7578954	7713024	94.22%	7.346%
40	13.133	1873	1878	1881	rBV3	263271	392594	4.80%	0.374%
41	13.215	1889	1892	1894	rBV3	214521	240477	2.94%	0.229%
42	13.239	1894	1896	1898	rVB	257128	216639	2.65%	0.206%
43	13.310	1906	1908	1910	rVB	137819	100417	1.23%	0.096%
44	13.345	1910	1914	1917	rBV2	372170	376349	4.60%	0.358%
45	13.374	1917	1919	1921	rVB	106265	83608	1.02%	0.080%
46	13.404	1921	1924	1927	rBV2	77796	92572	1.13%	0.088%
47	13.439	1927	1930	1932	rVB	213851	163281	1.99%	0.156%
48	13.468	1932	1935	1939	rBV2	202795	194845	2.38%	0.186%
49	13.633	1958	1963	1967	rBV6	126191	261149	3.19%	0.249%
50	13.745	1979	1982	1987	rVB	394681	367248	4.49%	0.350%
51	13.863	1997	2002	2004	rBV2	257682	368345	4.50%	0.351%
52	13.892	2004	2007	2008	rVV	255248	226109	2.76%	0.215%
53	13.910	2008	2010	2014	rVV2	298161	345728	4.22%	0.329%
54	13.951	2014	2017	2023	rVB2	1500962	1500653	18.33%	1.429%
55	14.115	2037	2045	2047	rBV2	2884392	4002781	48.90%	3.812%
56	14.139	2047	2049	2055	rVB	1309549	1161824	14.19%	1.107%
57	14.274	2070	2072	2078	rVB3	174934	256224	3.13%	0.244%
58	14.327	2078	2081	2086	rBV2	113373	125519	1.53%	0.120%
59	14.462	2102	2104	2106	rBV	101607	90148	1.10%	0.086%
60	14.498	2108	2110	2113	rVV	302295	248415	3.03%	0.237%
61	14.533	2113	2116	2120	rVB	296970	252188	3.08%	0.240%
62	14.586	2120	2125	2129	rBV4	274267	375610	4.59%	0.358%
63	14.627	2129	2132	2134	rBV2	139062	140524	1.72%	0.134%
64	14.810	2160	2163	2166	rBV2	81809	90732	1.11%	0.086%
65	14.904	2176	2179	2182	rVB3	206901	200627	2.45%	0.191%
66	14.986	2189	2193	2205	rVV3	843606	1025776	12.53%	0.977%
67	15.074	2205	2208	2212	rVB2	127136	137135	1.68%	0.131%
68	15.174	2220	2225	2228	rBV	1295565	1984724	24.24%	1.890%
69	15.257	2236	2239	2241	rBV2	197752	203519	2.49%	0.194%
70	15.286	2241	2244	2247	rVB	242920	245103	2.99%	0.233%
71	15.492	2275	2279	2285	rVB	721966	965755	11.80%	0.920%

LSC Area Percent Report

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Instrument : BNA_F
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Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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72	15.551	2285	2289	2296	rBV	708124	869139	10.62%	0.828%
73	15.621	2296	2301	2304	rVV	1864968	2271062	27.74%	2.163%
74	15.656	2304	2307	2313	rVB3	337245	525245	6.42%	0.500%
75	16.121	2382	2386	2391	rBV2	131691	217308	2.65%	0.207%
76	16.168	2391	2394	2398	rBV5	98795	154007	1.88%	0.147%
77	17.145	2554	2560	2567	rVB2	398017	778640	9.51%	0.742%
78	17.603	2632	2638	2648	rVB	309849	648575	7.92%	0.618%

Sum of corrected areas: 104999378

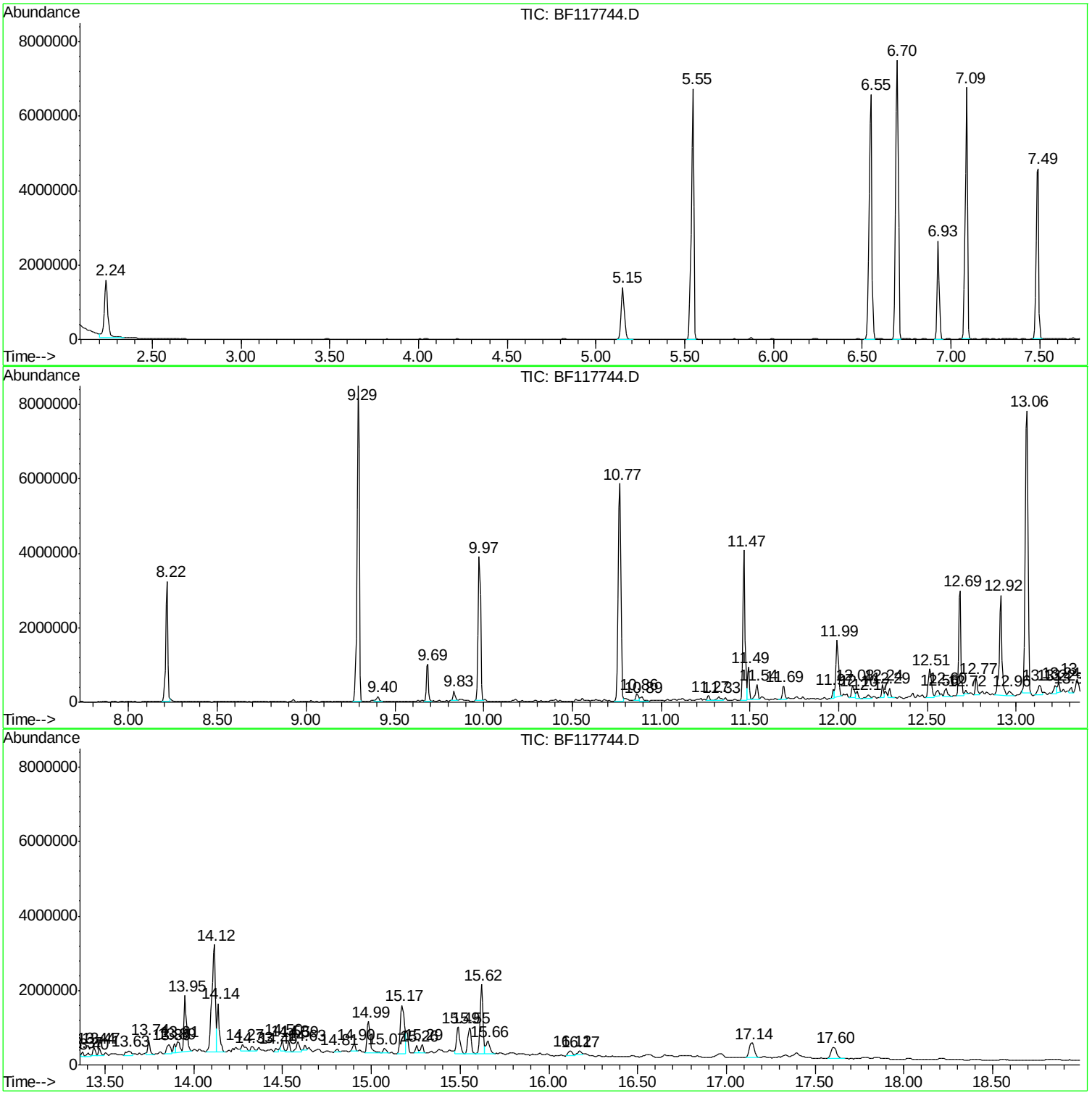
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110819\
Data File : BF117744.D
Acq On : 8 Nov 2019 21:10
Operator : JU
Sample : K5722-20
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.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\BF110819\
Data File : BF117744.D
Acq On : 8 Nov 2019 21:10
Operator : JU
Sample : K5722-20
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

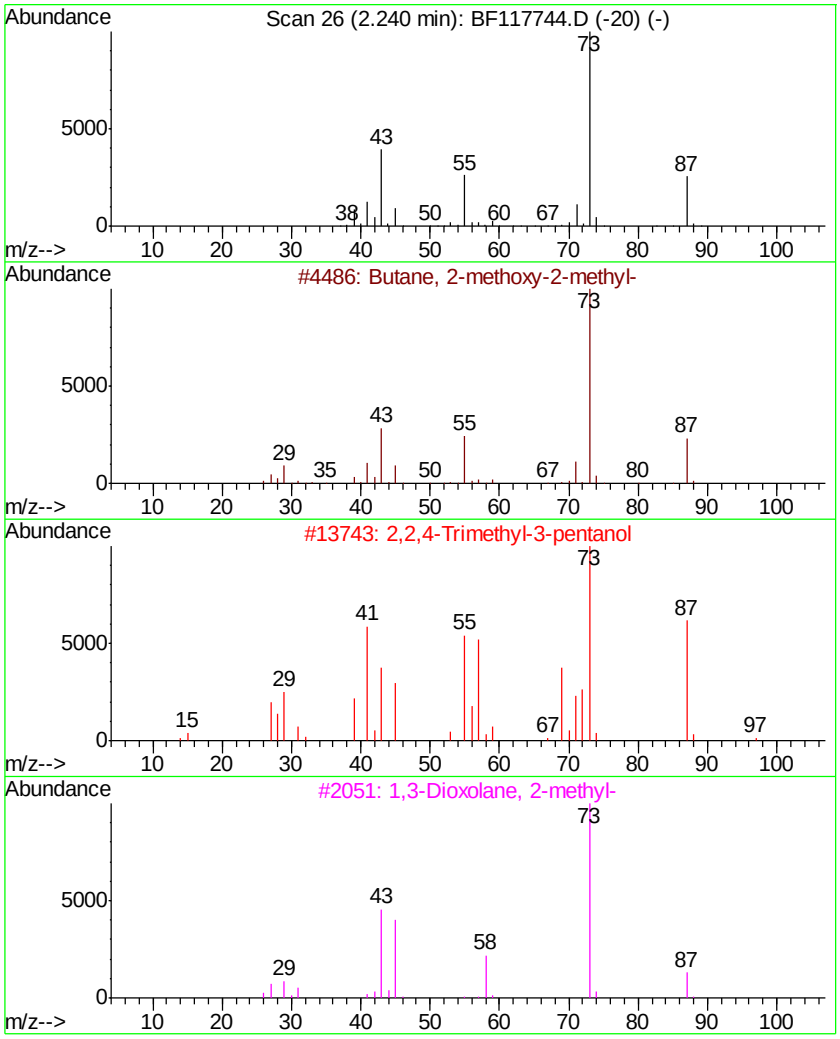
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

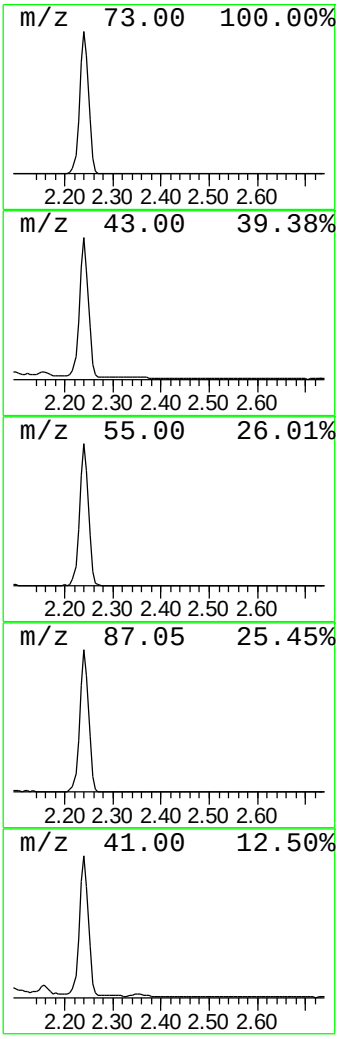
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.24	20.65 ng	2168290	1,4-Dichlorobenzene-d4	6.93

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	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10





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Acq On : 8 Nov 2019 21:10
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ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

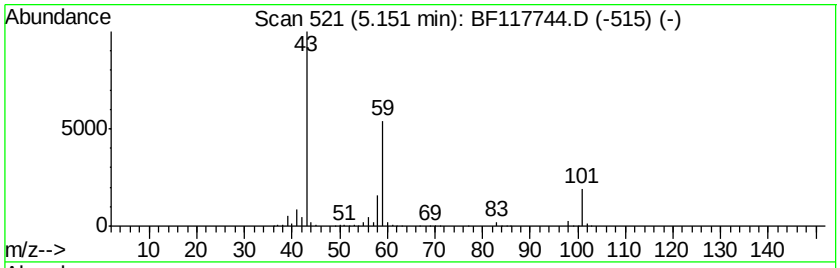
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

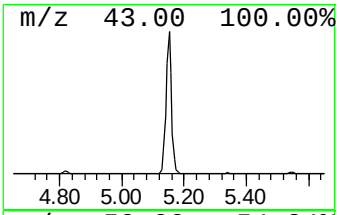
****

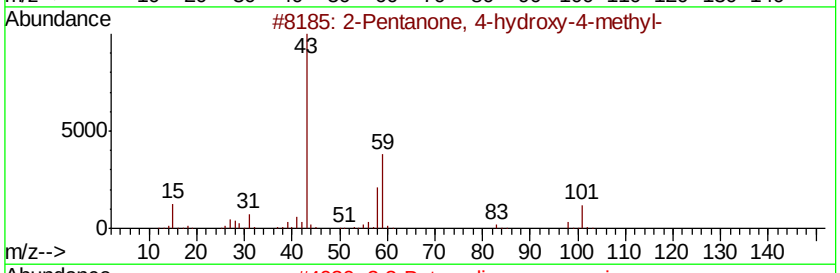
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

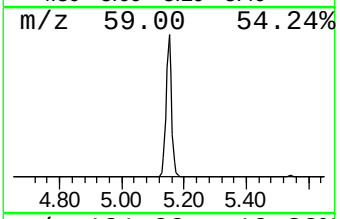
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	16.45 ng	1727190	1,4-Dichlorobenzene-d4	6.93

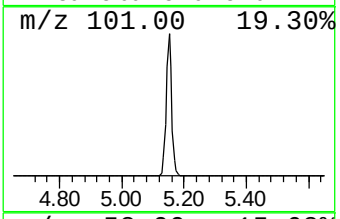
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9

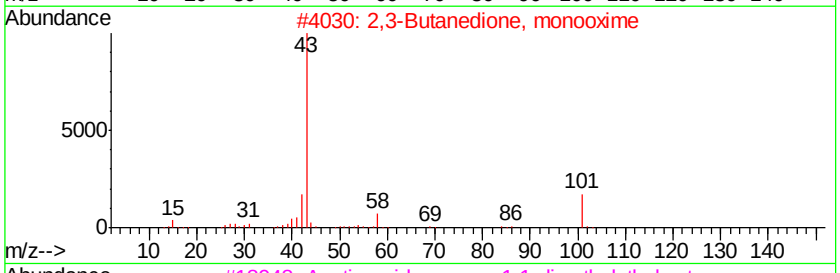


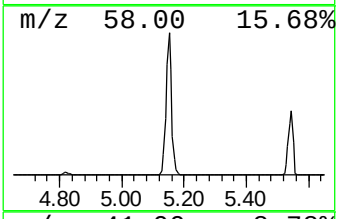


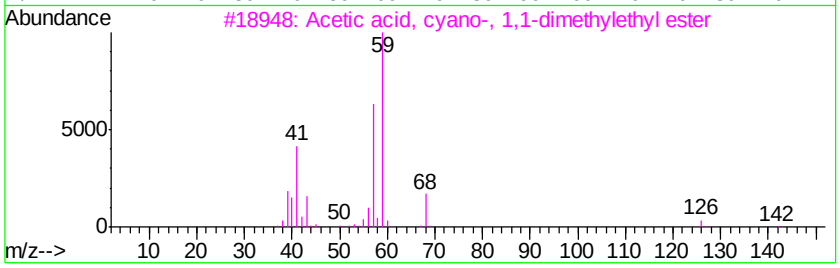


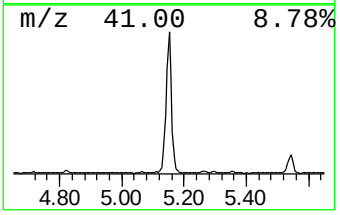












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

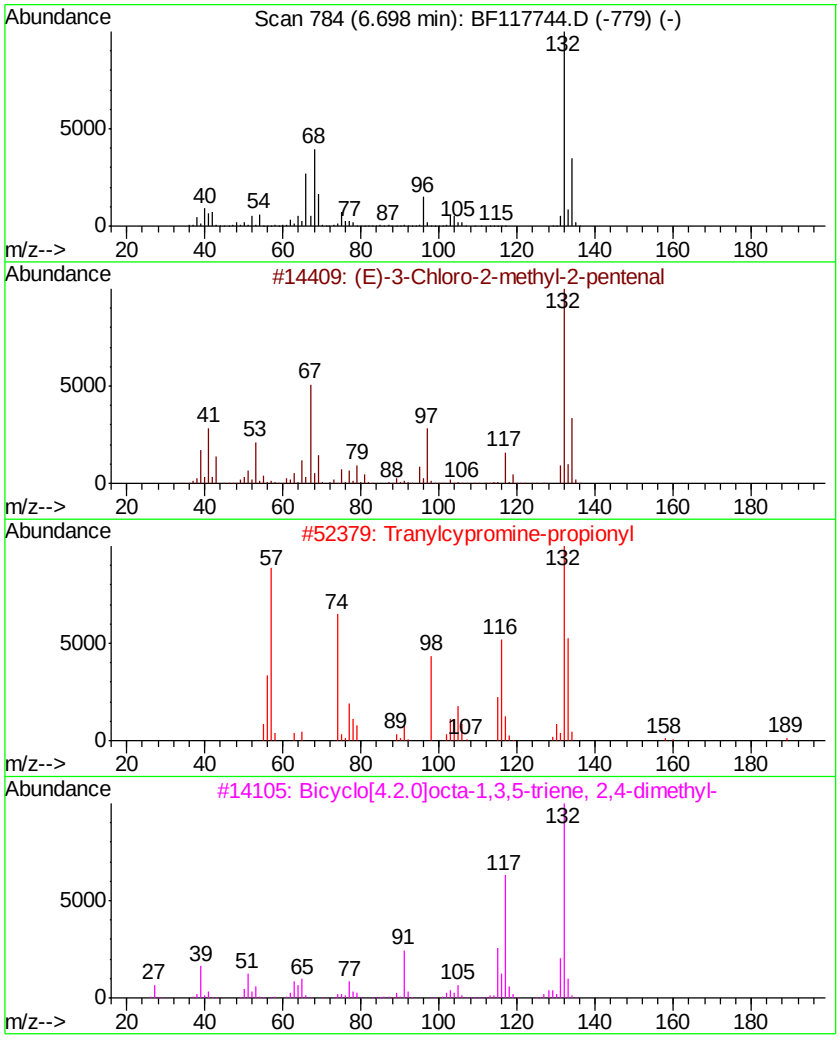
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

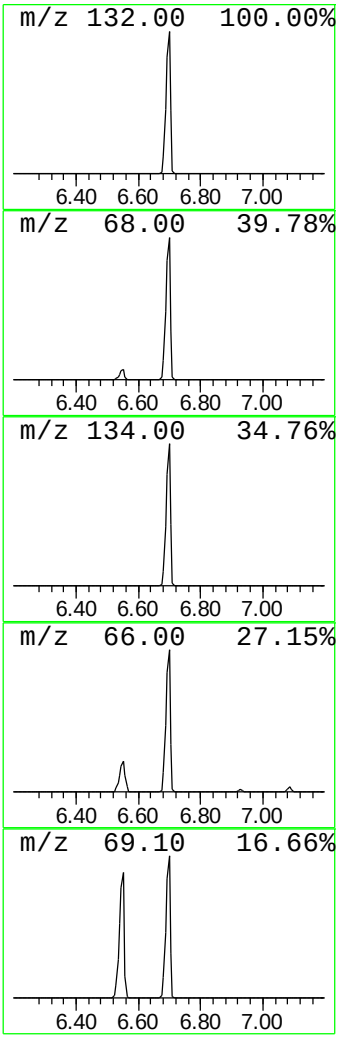
****

Peak Number 3 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	71.04 ng	7457750	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
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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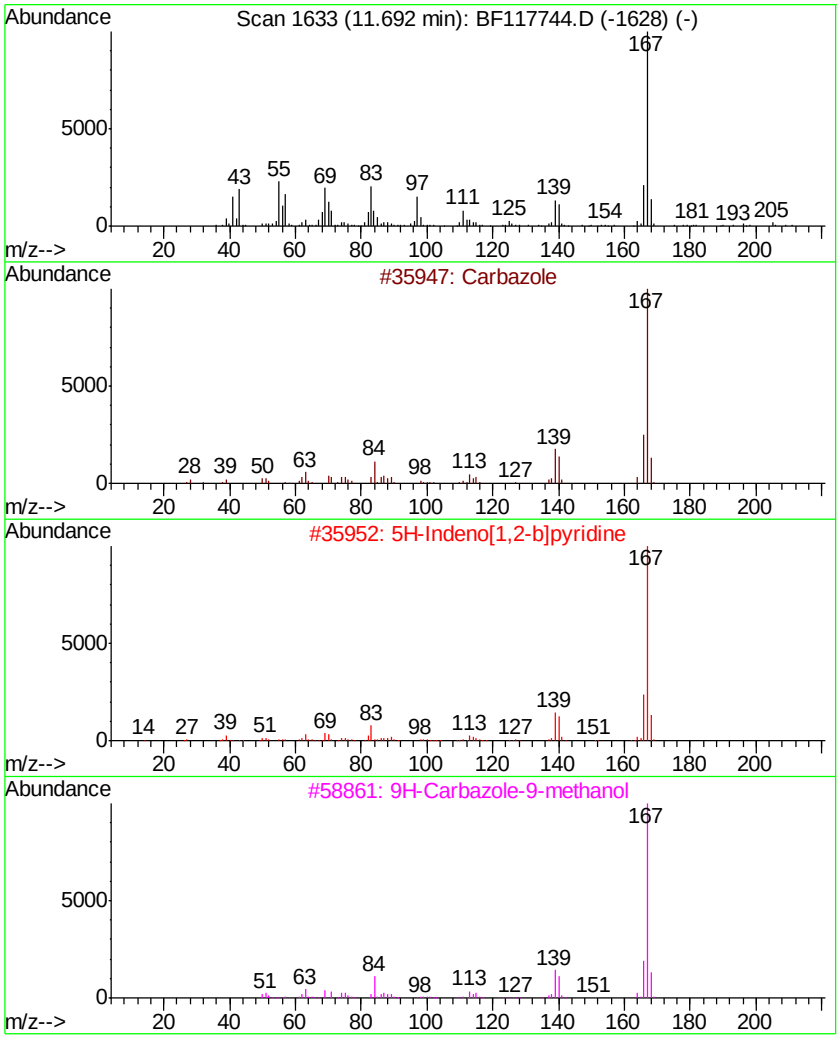
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

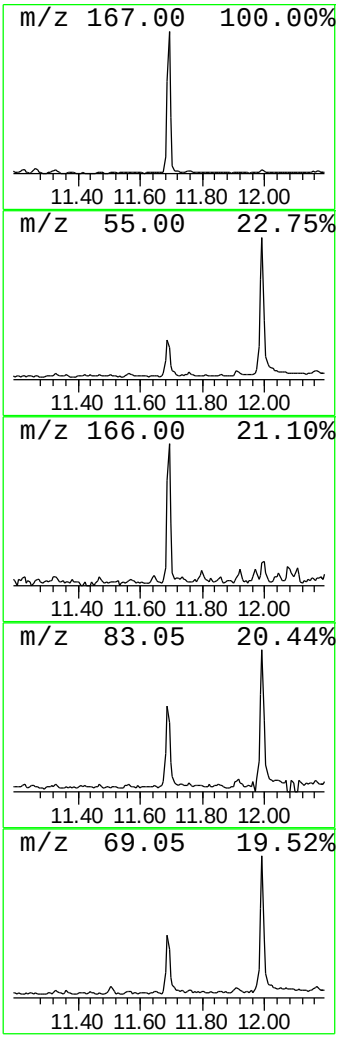
****

Peak Number 5 5H-Indeno[1,2-b]pyridine Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.69	2.35 ng	407445	Phenanthrene-d10	11.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbazole	167	C12H9N	000086-74-8	91
2	5H-Indeno[1,2-b]pyridine	167	C12H9N	000244-99-5	60
3	9H-Carbazole-9-methanol	197	C13H11NO	002409-36-1	53
4	D-Galactitol, 2-(acetylmethylami...	363	C16H29NO8	074410-42-7	47
5	2-Azafluorene	167	C12H9N	000244-40-6	43





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ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

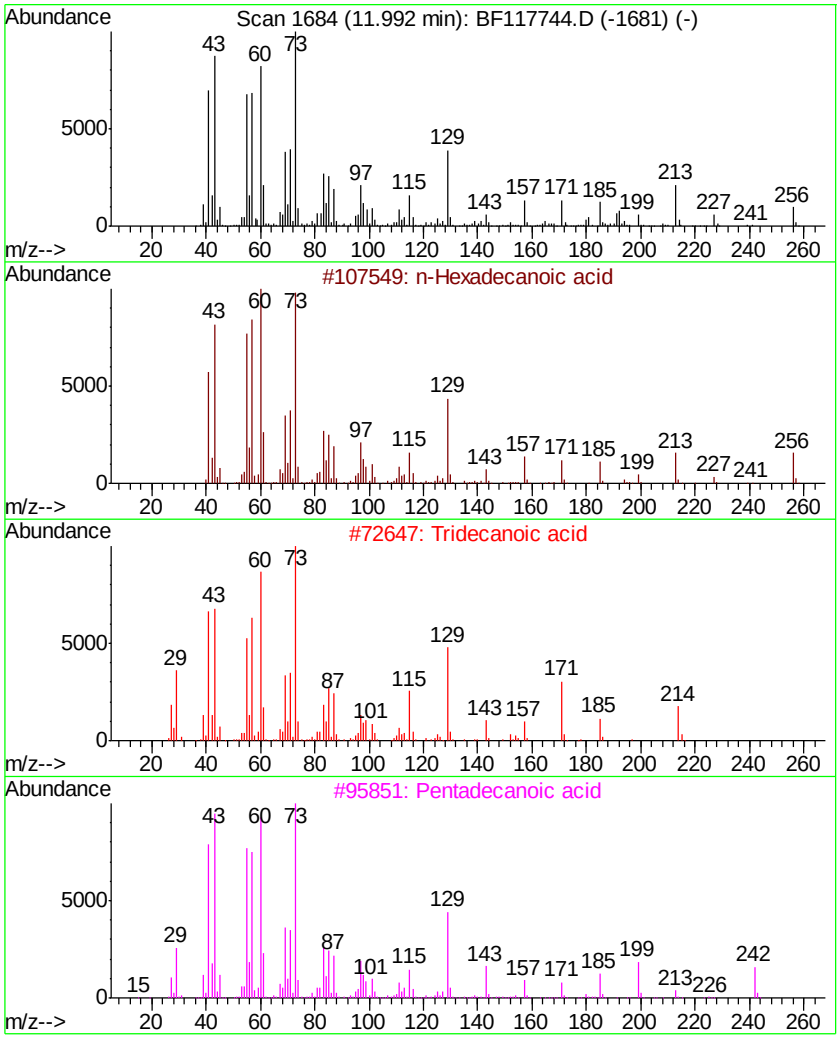
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

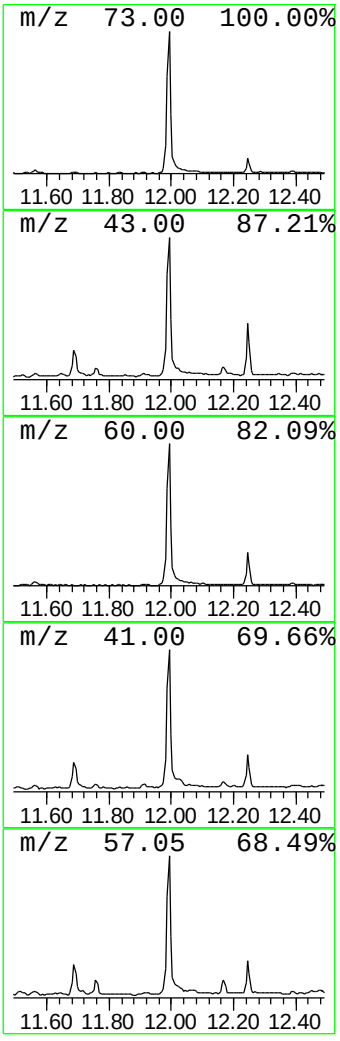
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	7.75 ng	1344770	Phenanthrene-d10	11.47

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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110819\
Data File : BF117744.D
Acq On : 8 Nov 2019 21:10
Operator : JU
Sample : K5722-20
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.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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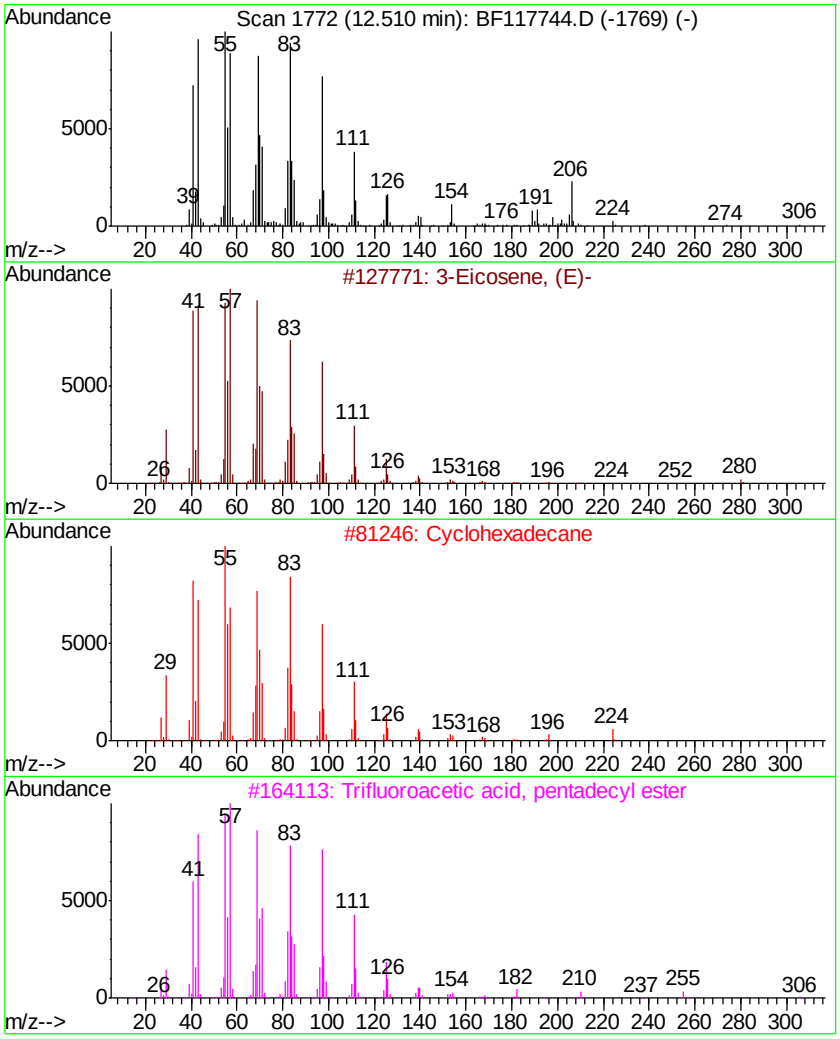
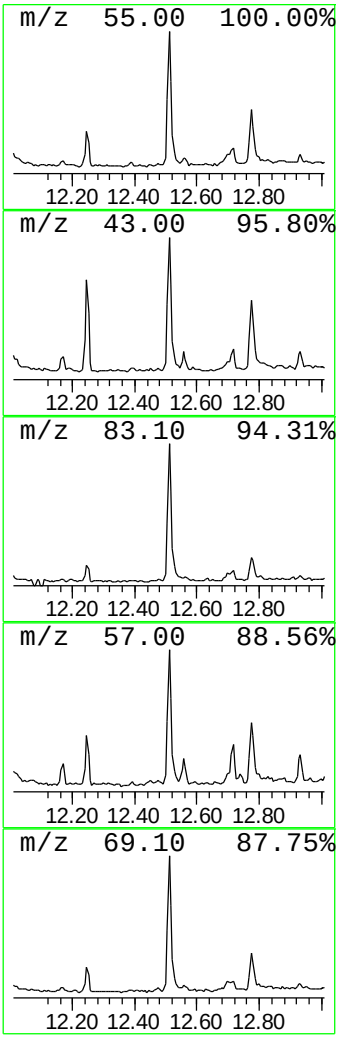
Peak Number 7 3-Eicosene, (E)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.51	5.04 ng	874012	Phenanthrene-d10	11.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	94
2	Cyclohexadecane	224	C16H32	000295-65-8	94
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
5	Trifluoroacetic acid,n-tridecyl ...	296	C15H27F3O2	053800-02-5	94





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Sample : K5722-20
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.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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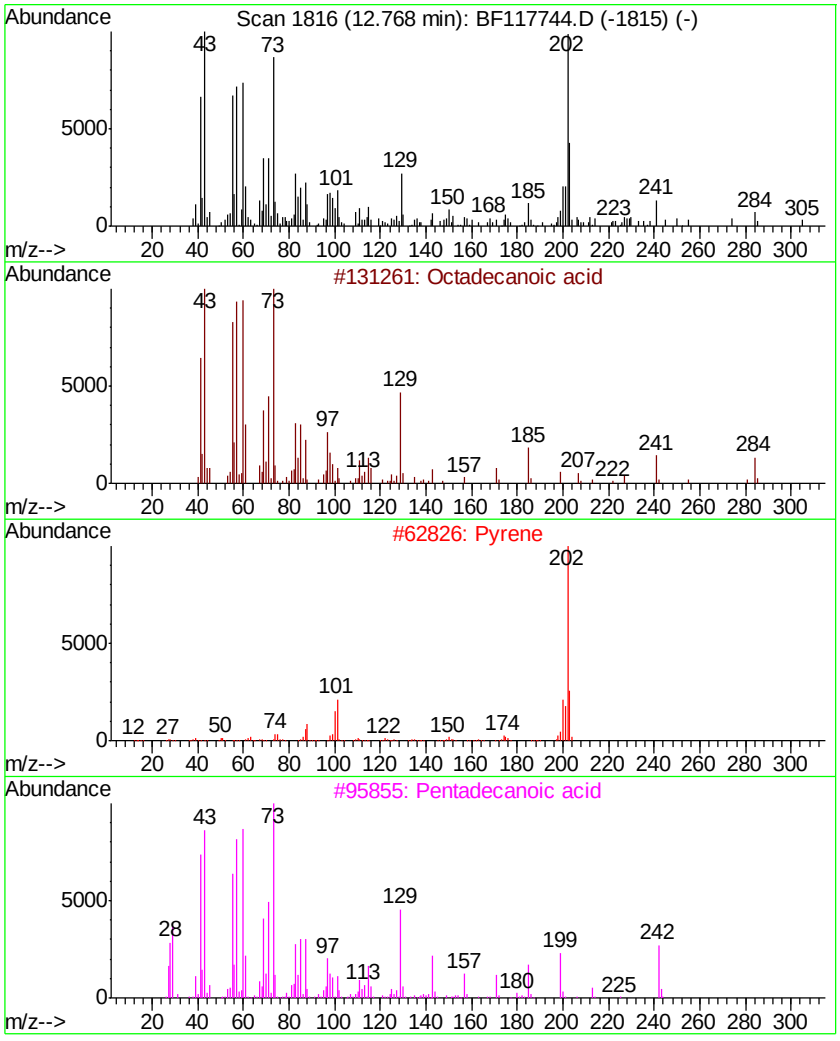
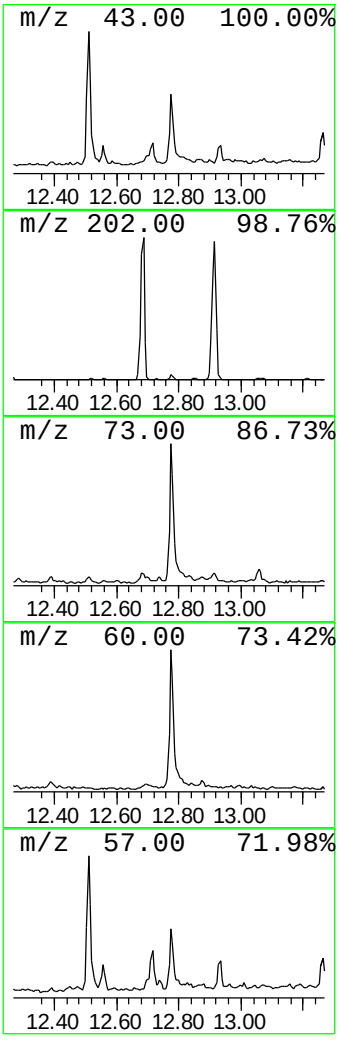
Peak Number 8 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	2.23 ng	386460	Phenanthrene-d10	11.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Pyrene	202	C16H10	000129-00-0	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Dodecanoic acid	200	C12H24O2	000143-07-7	50
5	Fluoranthene	202	C16H10	000206-44-0	42





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Operator : JU
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ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3-D

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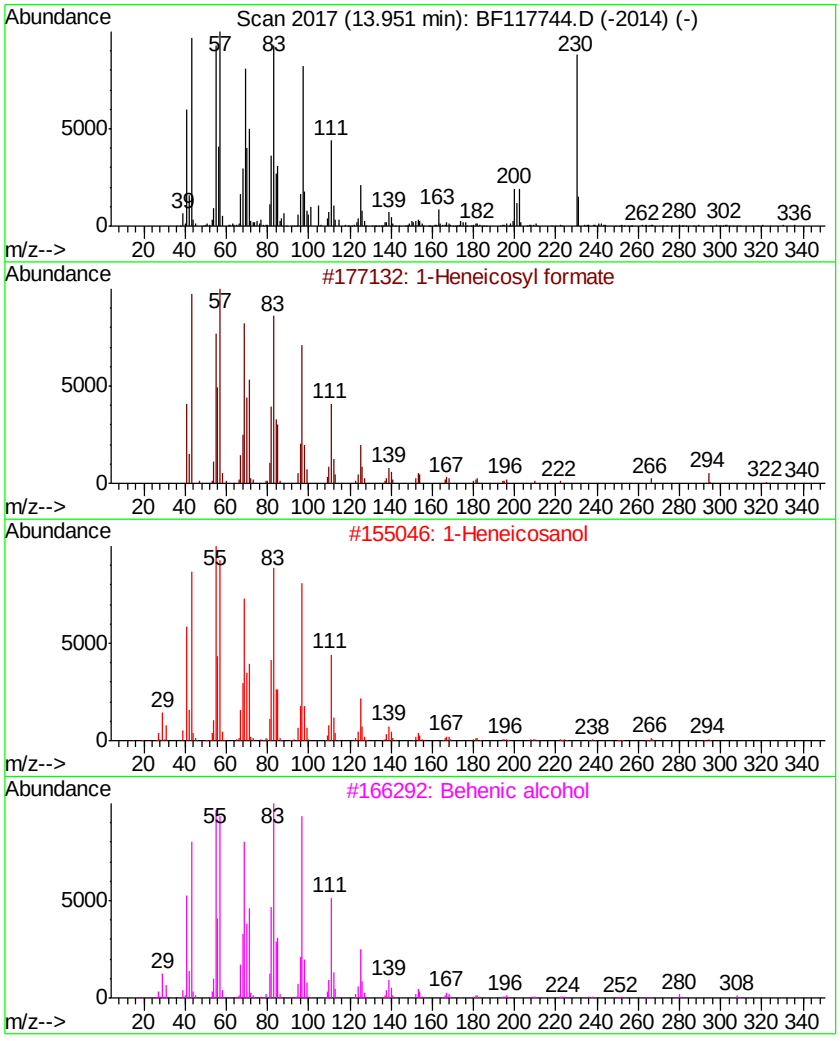
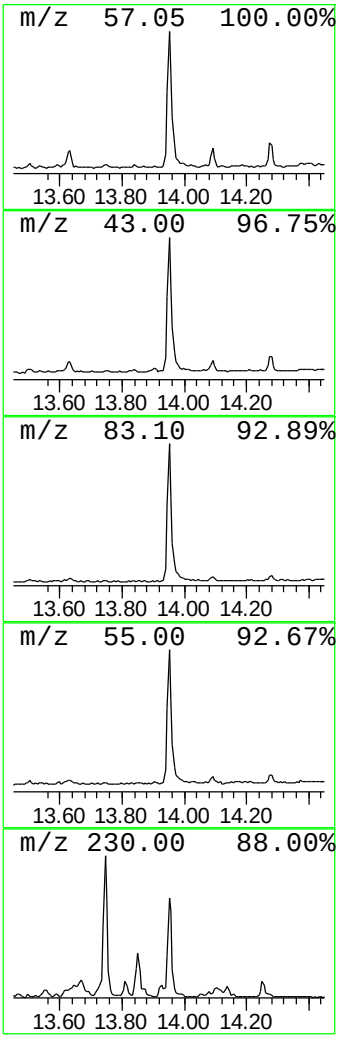
Peak Number 9 1-Heneicosyl formate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	7.50 ng	1500650	Chrysene-d12	14.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	86
2	1-Heneicosanol	312	C21H44O	015594-90-8	86
3	Behenic alcohol	326	C22H46O	000661-19-8	86
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	86
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	86





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Instrument : BNA_F
ClientSampleId : 3-D

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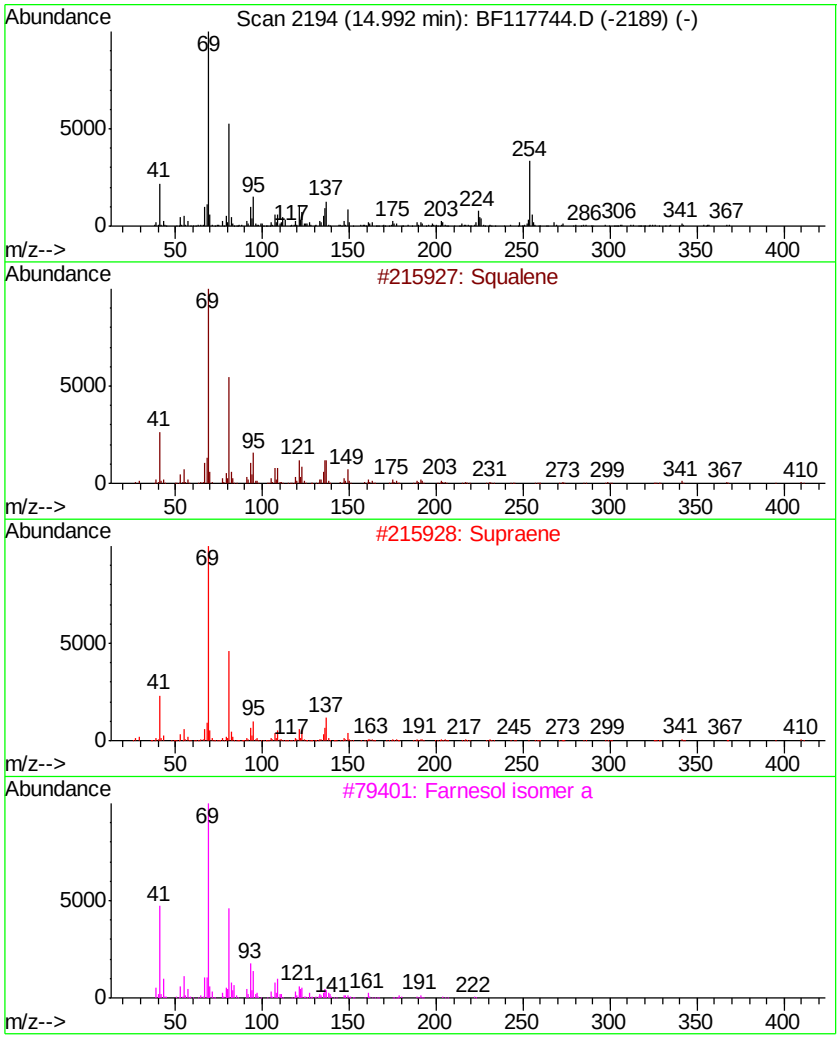
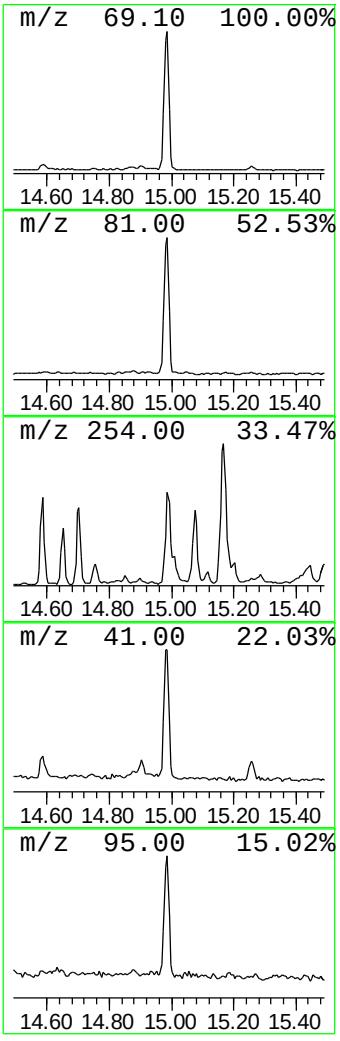
Peak Number 10 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	9.03 ng	1025780	Perylene-d12	15.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	92
2	Supraene	410	C30H50	007683-64-9	87
3	Farnesol isomer a	222	C15H26O	1000108-92-4	68
4	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	64
5	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	64





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Operator : JU
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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.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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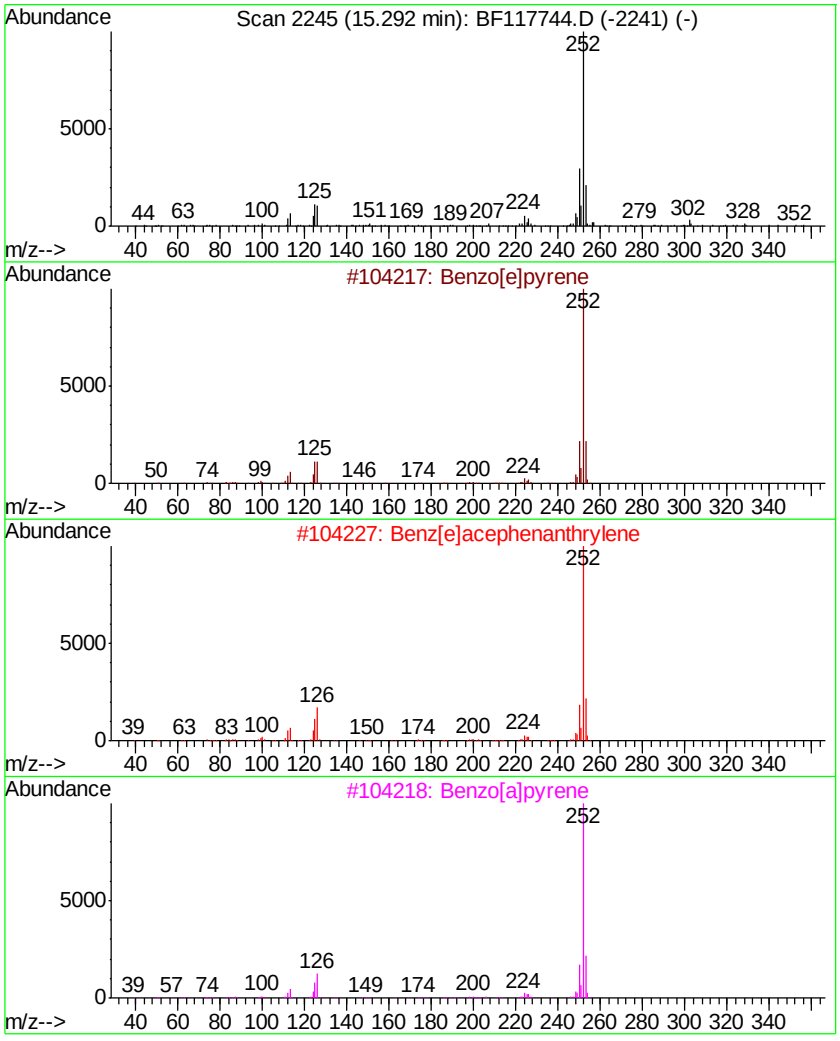
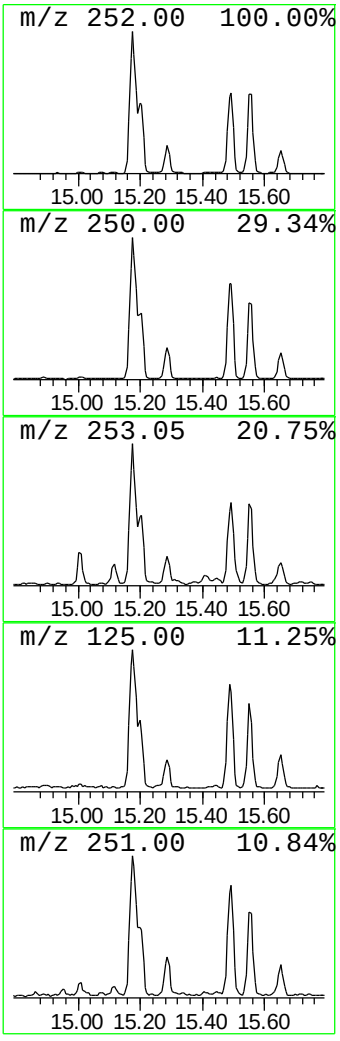
Peak Number 11 Benzo[e]pyrene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.29	2.16 ng	245103	Perylene-d12	15.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	97
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
3	Benzo[a]pyrene	252	C20H12	000050-32-8	91
4	Perylene	252	C20H12	000198-55-0	81
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	76





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Instrument : BNA_F
ClientSampleId : 3-D

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TIC Integration Parameters: LSCINT.P

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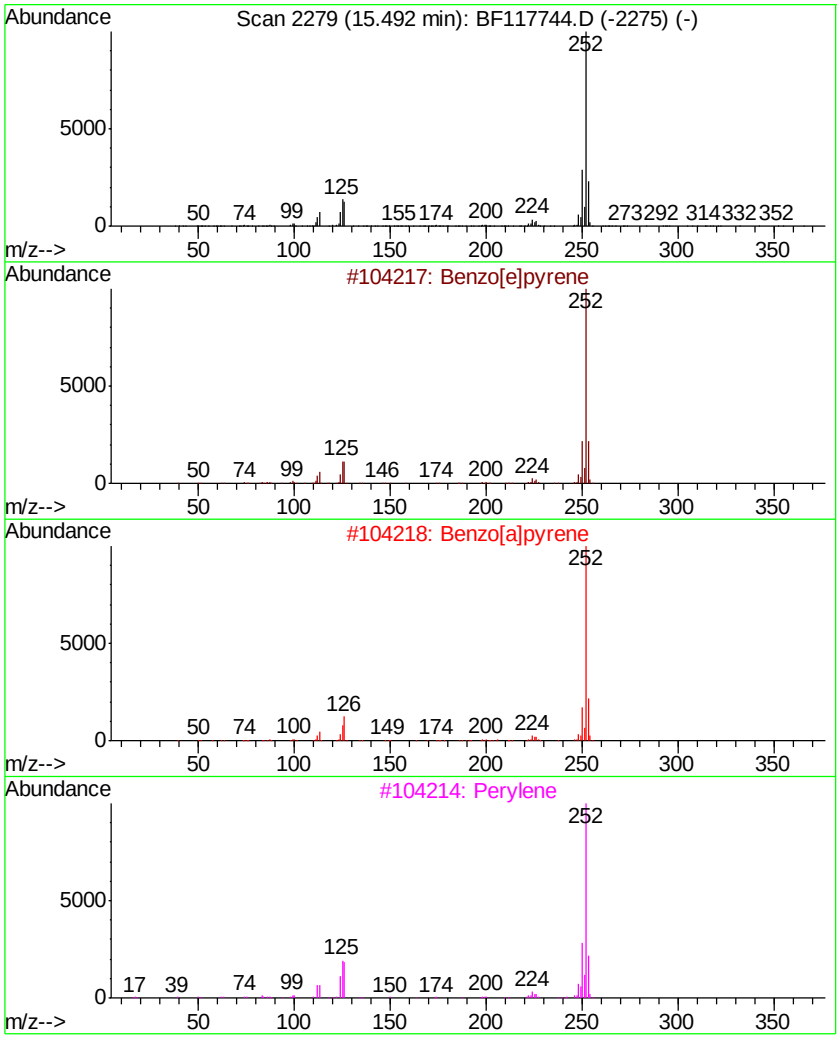
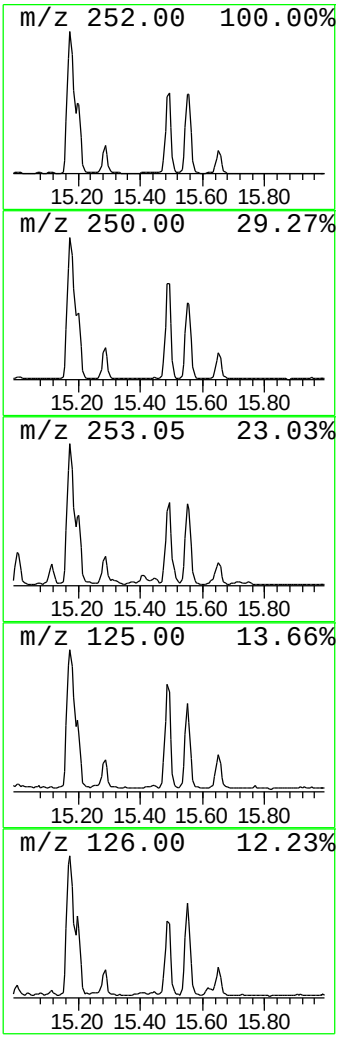
Peak Number 12 Perylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.49	8.50 ng	965755	Perylene-d12	15.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[a]pyrene	252	C20H12	000050-32-8	98
3	Perylene	252	C20H12	000198-55-0	96
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	94





Tentatively Identified Compound (LSC) summary

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Data File : BF117744.D
Acq On : 8 Nov 2019 21:10
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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3-D

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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
Butane, 2-methoxy...	2.24	20.6	ng	2168290	1	6.93	2099700	20.0
2-Pentanone, 4-hy...	5.15	16.4	ng	1727190	1	6.93	2099700	20.0
unknown6.70	6.70	71.0	ng	7457750	1	6.93	2099700	20.0
5H-Indeno[1,2-b]p...	11.69	2.4	ng	407445	4	11.47	3469890	20.0
n-Hexadecanoic acid	11.99	7.8	ng	1344770	4	11.47	3469890	20.0
3-Eicosene, (E)-	12.51	5.0	ng	874012	4	11.47	3469890	20.0
Octadecanoic acid	12.77	2.2	ng	386460	4	11.47	3469890	20.0
1-Heneicosyl formate	13.95	7.5	ng	1500650	5	14.12	4002780	20.0
Squalene	14.99	9.0	ng	1025780	6	15.62	2271060	20.0
Benzo[e]pyrene	15.29	2.2	ng	245103	6	15.62	2271060	20.0
Perylene	15.49	8.5	ng	965755	6	15.62	2271060	20.0