LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061021\
Data File : BF124246.D
Acq On : 10 Jun 2021 22:33
Operator : JU/CG
Sample : M2651-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 17-B6(0-4)

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-BF060321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124246.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	13	17	23	rBB2	10791	14835	1.88%	0.182%
2	5.057	501	505	512	rVB	35512	37778	4.78%	0.465%
3	5.475	573	576	585	rBV	690535	584776	73.94%	7.194%
4	5.681	608	611	617	rBV	24756	22820	2.89%	0.281%
5	6.487	744	748	758	rBV	706557	613994	77.64%	7.553%
6	6.681	777	781	785	rBV2	41872	43721	5.53%	0.538%
7	6.722	785	788	791	rVB2	12957	11151	1.41%	0.137%
8	6.845	806	809	813	rBV	304308	227205	28.73%	2.795%
9	7.110	851	854	861	rBB2	18953	18858	2.38%	0.232%
10	7.410	900	905	908	rBV	490781	412509	52.16%	5.074%
11	7.698	952	954	962	rVB	30270	30500	3.86%	0.375%
12	8.128	1024	1027	1033	rVB	377275	295050	37.31%	3.630%
13	8.345	1061	1064	1067	rBV	25531	20342	2.57%	0.250%
14	8.404	1071	1074	1078	rVV3	26695	22374	2.83%	0.275%
15	8.839	1145	1148	1151	rBV	14571	15319	1.94%	0.188%
16	9.204	1206	1210	1213	rBV	1025414	790863	100.00%	9.729%
17	9.334	1226	1232	1241	rBV	74425	101947	12.89%	1.254%
18	9.598	1274	1277	1280	rBV	181749	132293	16.73%	1.627%
19	9.828	1311	1316	1318	rBV3	23002	26342	3.33%	0.324%
20	9.857	1318	1321	1323	rVV3	15005	20147	2.55%	0.248%
21	9.886	1323	1326	1329	rVV	443575	351679	44.47%	4.326%
22	9.916	1329	1331	1334	rVB	33517	25250	3.19%	0.311%
23	10.428	1416	1418	1421	rVB2	16751	15810	2.00%	0.194%
24	10.675	1456	1460	1465	rBV	658370	543550	68.73%	6.686%
25	10.851	1486	1490	1495	rBV7	7976	11738	1.48%	0.144%
26	11.269	1558	1561	1564	rVB2	13110	11010	1.39%	0.135%
27	11.375	1575	1579	1581	rBV	387219	361566	45.72%	4.448%
28	11.392	1581	1582	1586	rVV	164923	130383	16.49%	1.604%
29	11.445	1589	1591	1594	rVB	42485	32177	4.07%	0.396%
30	11.604	1612	1618	1621	rBV4	15462	22747	2.88%	0.280%
31	11.875	1661	1664	1665	rBV3	15492	13802	1.75%	0.170%
32	11.898	1665	1668	1672	rVB2	73271	67082	8.48%	0.825%
33	11.986	1679	1683	1685	rBV	31644	32385	4.09%	0.398%
34	12.010	1685	1687	1689	rVB3	15809	12044	1.52%	0.148%
35	12.169	1711	1714	1717	rBV2	16009	17810	2.25%	0.219%
36	12.198	1717	1719	1724	rVB5	14032	13672	1.73%	0.168%

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Sample : M2651-04
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Instrument : BNA_F
ClientSampleId : 17-B6(0-4)

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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37	12.422	1755	1757	1760	rBV3	14660	15864	2.01%	0.195%
38	12.510	1769	1772	1777	rVB5	14460	15514	1.96%	0.191%
39	12.586	1781	1785	1788	rBV	234128	191683	24.24%	2.358%
40	12.680	1798	1801	1804	rBV3	21950	24583	3.11%	0.302%
41	12.816	1818	1824	1829	rBV	198535	216294	27.35%	2.661%
42	12.874	1832	1834	1838	rVB4	13252	12372	1.56%	0.152%
43	12.957	1844	1848	1851	rBV	776366	647951	81.93%	7.971%
44	13.033	1856	1861	1865	rBV7	23633	35077	4.44%	0.431%
45	13.116	1871	1875	1877	rBV5	12351	14472	1.83%	0.178%
46	13.145	1877	1880	1883	rVB2	23755	24415	3.09%	0.300%
47	13.210	1889	1891	1894	rVB2	17021	13505	1.71%	0.166%
48	13.245	1894	1897	1899	rBV4	19600	19403	2.45%	0.239%
49	13.339	1911	1913	1916	rBV2	18754	16679	2.11%	0.205%
50	13.369	1916	1918	1921	rVB3	15890	13564	1.72%	0.167%
51	13.433	1926	1929	1934	rVB3	36052	33777	4.27%	0.416%
52	13.651	1963	1966	1970	rVB3	18676	20976	2.65%	0.258%
53	13.763	1980	1985	1988	rBV4	18107	24754	3.13%	0.305%
54	13.792	1988	1990	1992	rVV2	21432	15851	2.00%	0.195%
55	13.827	1992	1996	1998	rVV4	10715	17175	2.17%	0.211%
56	13.857	1998	2001	2012	rVB5	58131	97150	12.28%	1.195%
57	14.016	2020	2028	2031	rBV2	325108	421487	53.29%	5.185%
58	14.039	2031	2032	2038	rVB	96202	68501	8.66%	0.843%
59	14.121	2043	2046	2050	rVB5	16236	15800	2.00%	0.194%
60	14.239	2064	2066	2070	rVB5	12334	12093	1.53%	0.149%
61	14.404	2090	2094	2097	rVB	32497	33050	4.18%	0.407%
62	14.433	2097	2099	2104	rBV4	17271	16304	2.06%	0.201%
63	14.480	2104	2107	2108	rBV3	17285	13078	1.65%	0.161%
64	14.498	2108	2110	2112	rVB3	17772	11971	1.51%	0.147%
65	14.521	2112	2114	2116	rBV3	16387	18049	2.28%	0.222%
66	14.586	2123	2125	2130	rVB6	10744	16875	2.13%	0.208%
67	14.716	2144	2147	2150	rVB5	9738	12284	1.55%	0.151%
68	14.786	2156	2159	2160	rBV3	10770	11606	1.47%	0.143%
69	15.063	2201	2206	2213	rBV2	89247	178268	22.54%	2.193%
70	15.168	2222	2224	2228	rVB3	18955	15057	1.90%	0.185%
71	15.257	2238	2239	2244	rBV5	10333	17183	2.17%	0.211%
72	15.316	2247	2249	2253	rVB4	10829	12823	1.62%	0.158%
73	15.363	2253	2257	2264	rVB	57327	79730	10.08%	0.981%
74	15.427	2264	2268	2275	rVB2	84341	105629	13.36%	1.299%
75	15.492	2275	2279	2287	rBV	232761	313785	39.68%	3.860%
76	15.827	2329	2336	2339	rBV8	12358	22988	2.91%	0.283%

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Sample : M2651-04
Misc :
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Instrument : BNA_F
ClientSampleId : 17-B6(0-4)

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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	15.939	2352	2355	2358	rVB4	13280	17473	2.21%	0.215%
78	16.027	2367	2370	2372	rBV4	10715	12243	1.55%	0.151%
79	16.968	2526	2530	2539	rVB3	32843	72392	9.15%	0.891%
80	17.421	2601	2607	2612	rVB6	19462	40050	5.06%	0.493%
81	17.857	2675	2681	2684	rBV7	6438	13797	1.74%	0.170%

Sum of corrected areas: 8129104

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061021\
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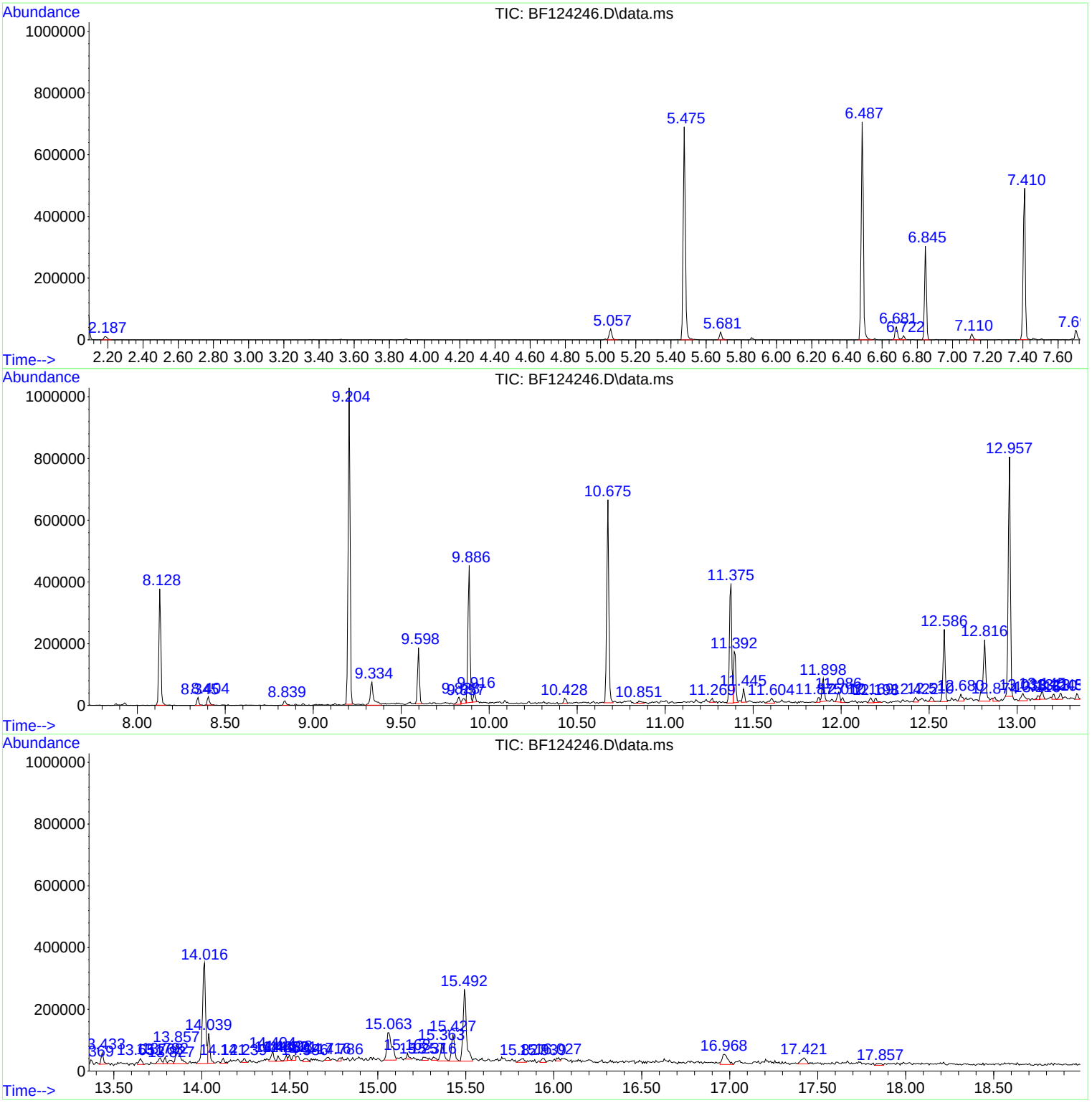
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
17-B6(0-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061021\
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Sample : M2651-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
17-B6(0-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

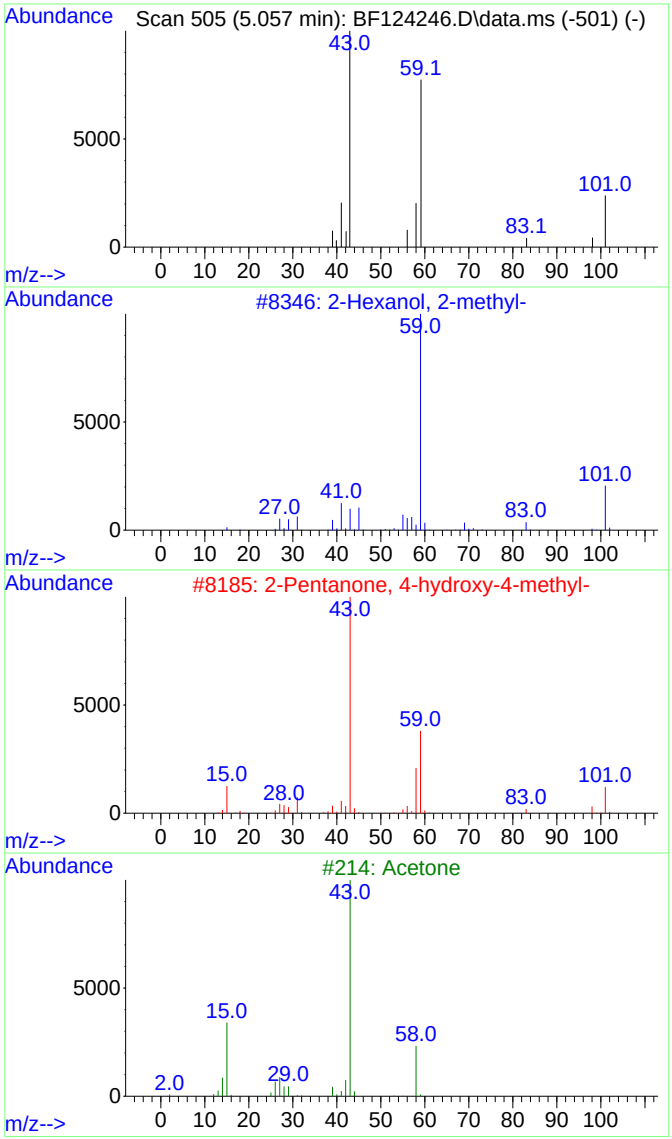
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

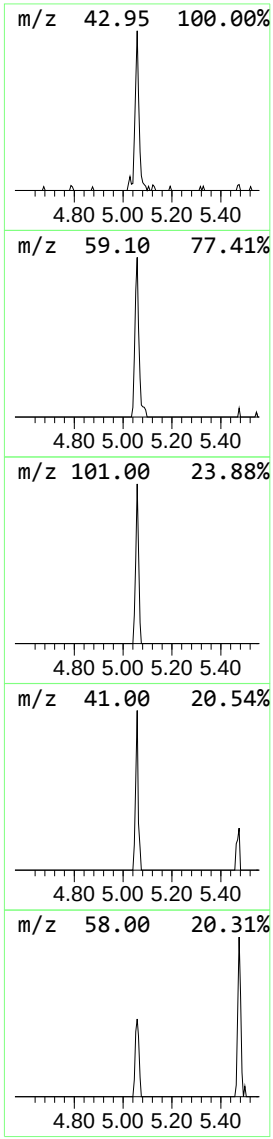
****

Peak Number 1 unknown5.057 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	3.33 ng	37778	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	9
3	Acetone	58	C3H6O	000067-64-1	7
4	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	5
5	2-Propanone, 1-cyclopropyl-	98	C6H10O	004160-75-2	5





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Sample : M2651-04
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Instrument :
BNA_F
ClientSampleId :
17-B6(0-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

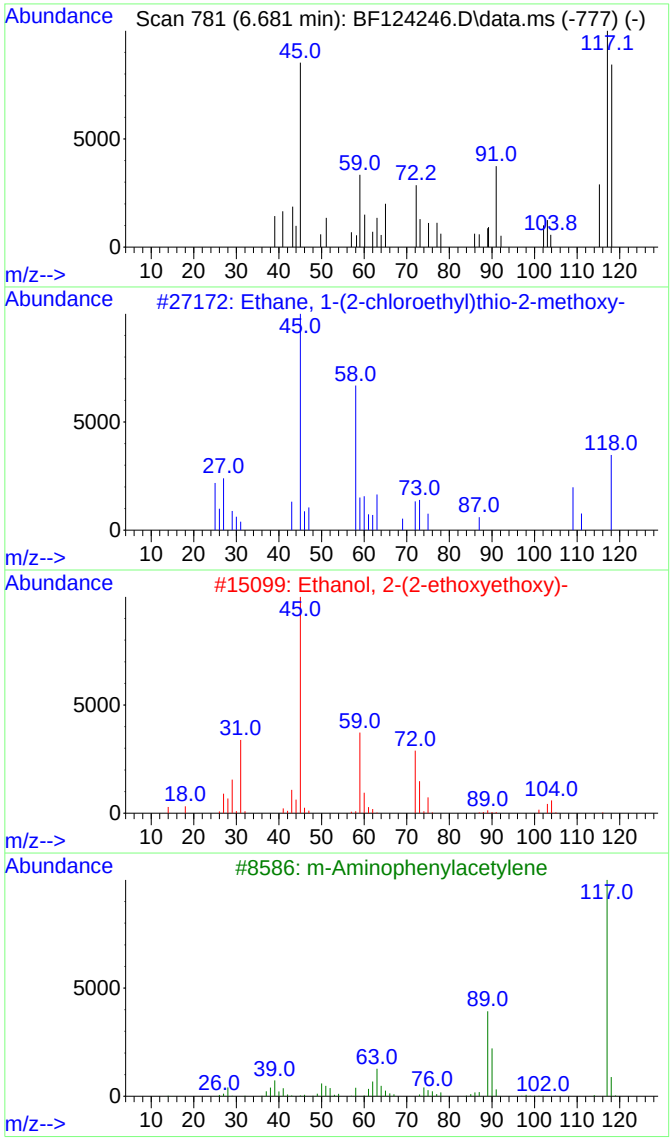
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

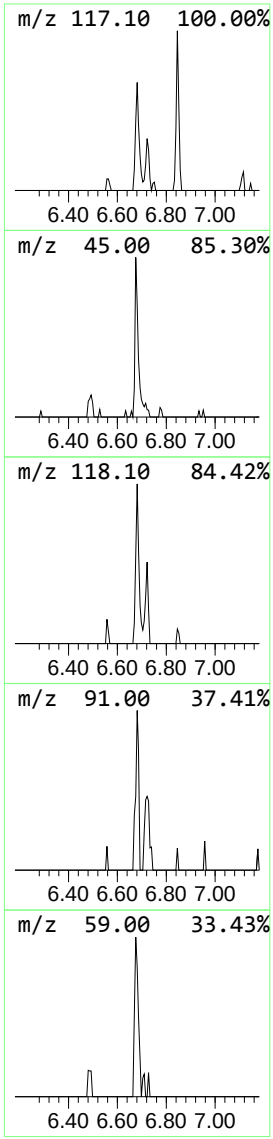
****

Peak Number 3 unknown6.681 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.681	3.85 ng	43721	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethane, 1-(2-chloroethyl)thio-2-...	154	C5H11ClOS	091159-34-1	37
2	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	22
3	m-Aminophenylacetylene	117	C8H7N	054060-30-9	14
4	1,3-Methanopentalene, 1,2,3,5-te...	118	C9H10	128600-88-4	12
5	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	12





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ClientSampleId :
17-B6(0-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
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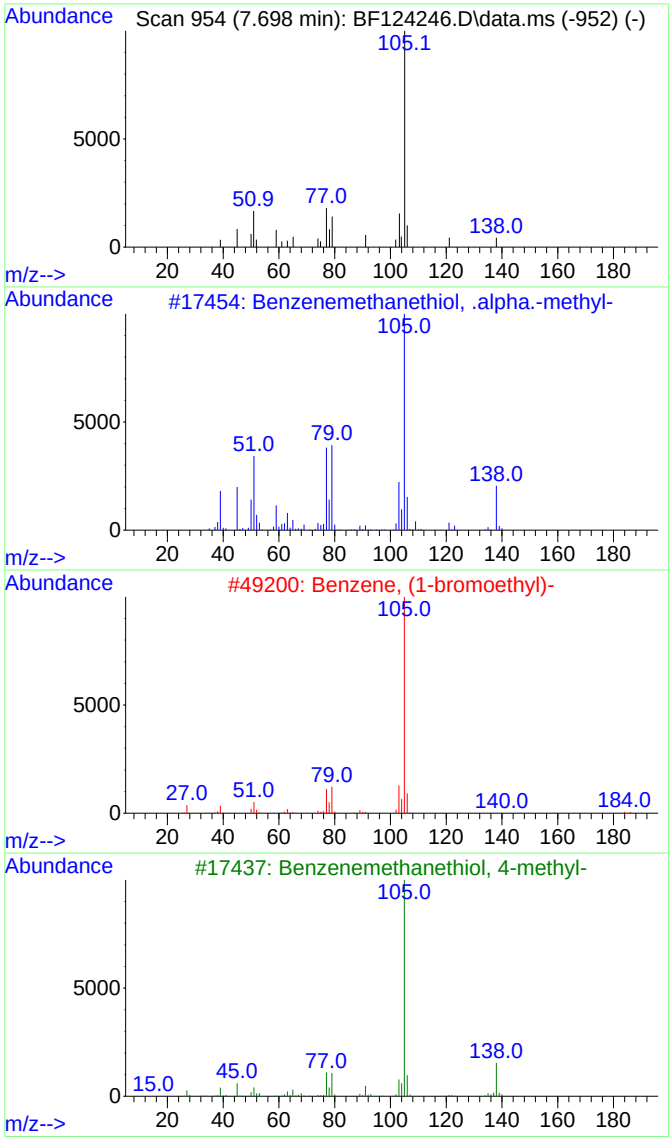
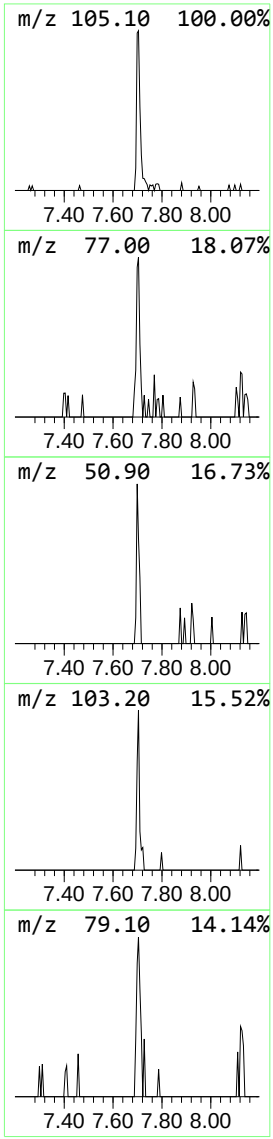
****
Peak Number 4 Benzenemethanethiol, .alpha... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.698	2.07 ng	30500	Naphthalene-d8	8.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenemethanethiol, .alpha.-met...	138	C8H10S	006263-65-6	72
2	Benzene, (1-bromoethyl)-	184	C8H9Br	000585-71-7	64
3	Benzenemethanethiol, 4-methyl-	138	C8H10S	004498-99-1	59
4	Ether, p-methylbenzyl vinyl	148	C10H12O	026437-10-5	59
5	3-Phenylpropanoic anhydride	282	C18H18O3	1000333-89-6	53





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TIC Library : C:\DATABASE\NIST11.L
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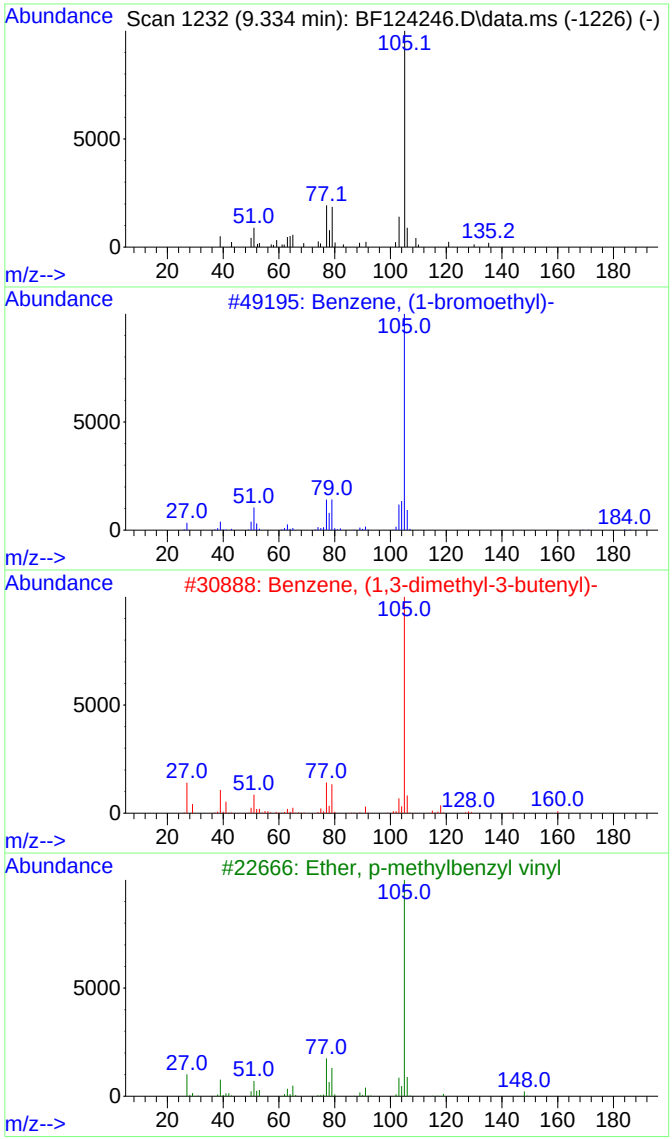
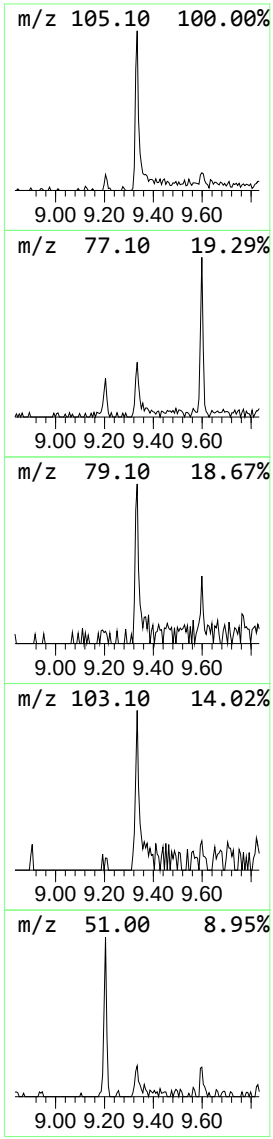
****
Peak Number 5 Benzene, (1-bromoethyl)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.334	5.80 ng	101947	Acenaphthene-d10	9.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-bromoethyl)-	184	C8H9Br	000585-71-7	59
2	Benzene, (1,3-dimethyl-3-butenyl)-	160	C12H16	056851-51-5	59
3	Ether, p-methylbenzyl vinyl	148	C10H12O	026437-10-5	59
4	Benzene, (1-nitroethyl)-	151	C8H9NO2	007214-61-1	59
5	Benzene, 1,1'-(oxydiethylidene)bis-	226	C16H18O	000093-96-9	53





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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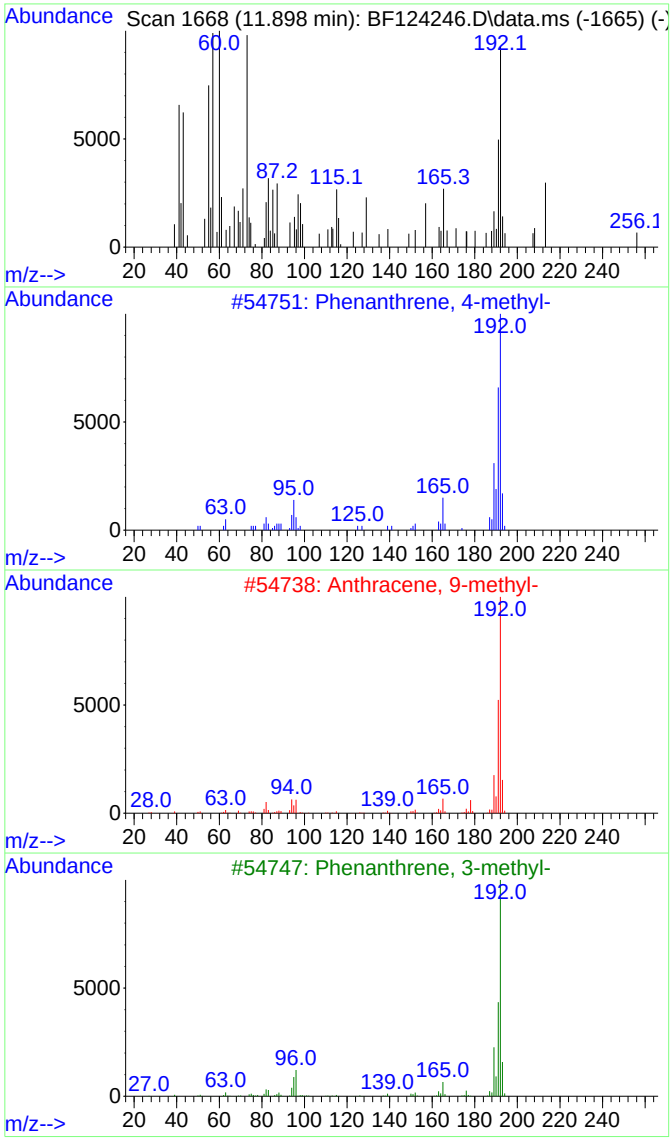
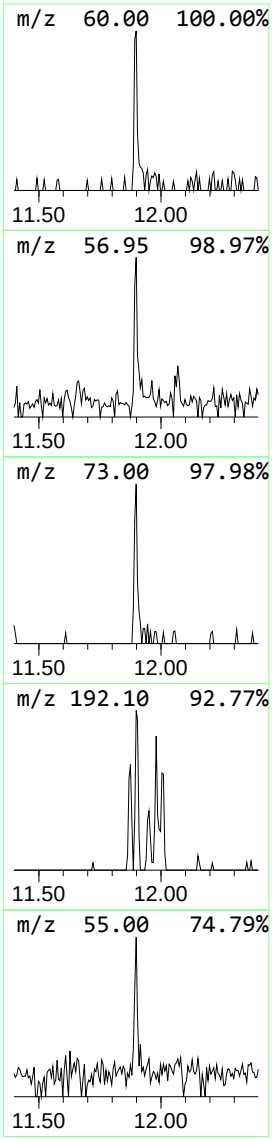
Peak Number 6 unknown11.898 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	3.71 ng	67082	Phenanthrene-d10	11.375

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	42
2	Anthracene, 9-methyl-	192	C15H12	000779-02-2	42
3	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	42
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	42
5	Phenanthrene, 9-methyl-	192	C15H12	000883-20-5	42





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Data File : BF124246.D
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Operator : JU/CG
Sample : M2651-04
Misc :
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Instrument : BNA_F
ClientSampleId : 17-B6(0-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.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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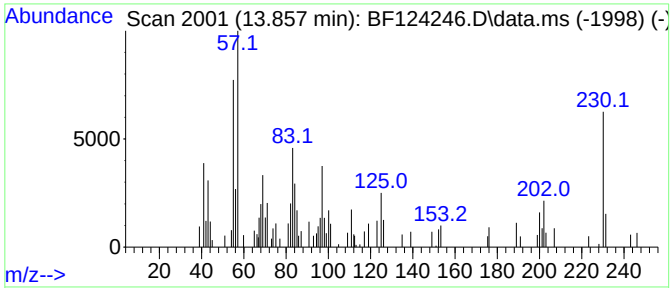
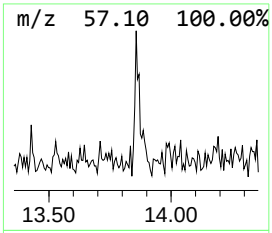
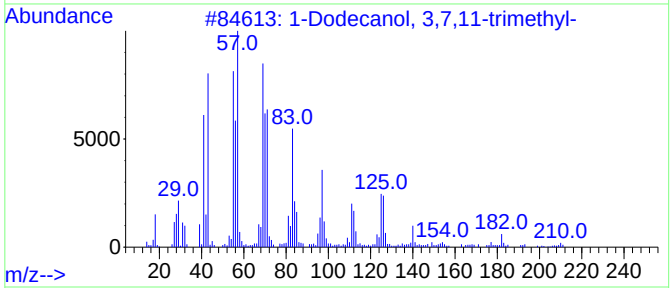
Peak Number 7 unknown13.857 Concentration Rank 3

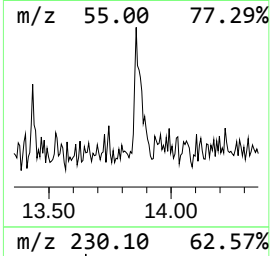
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	4.61 ng	97150	Chrysene-d12	14.016

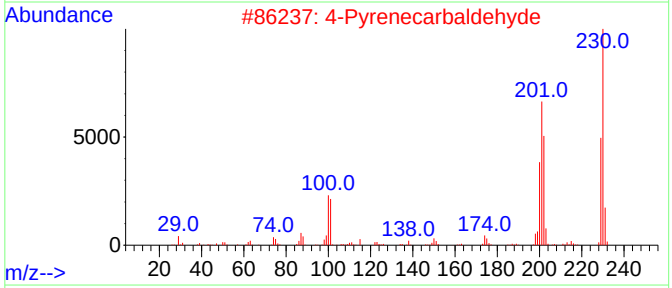
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 3,7,11-trimethyl-	228	C15H32O	006750-34-1	35
2	4-Pyrenecarbaldehyde	230	C17H10O	022245-51-8	30
3	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	30
4	Pentafluoropropionic acid, undec...	318	C14H23F5O2	959014-11-0	30
5	Trichloroacetic acid, undecyl ester	316	C13H23Cl3O2	074339-49-4	30

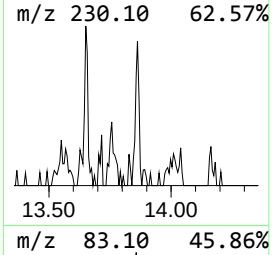


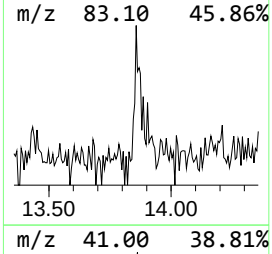


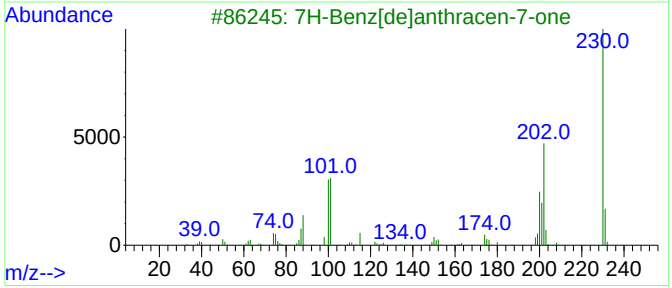


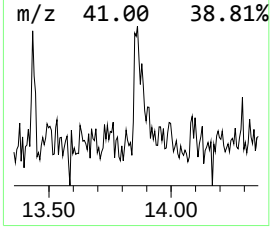












Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061021\
Data File : BF124246.D
Acq On : 10 Jun 2021 22:33
Operator : JU/CG
Sample : M2651-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
17-B6(0-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

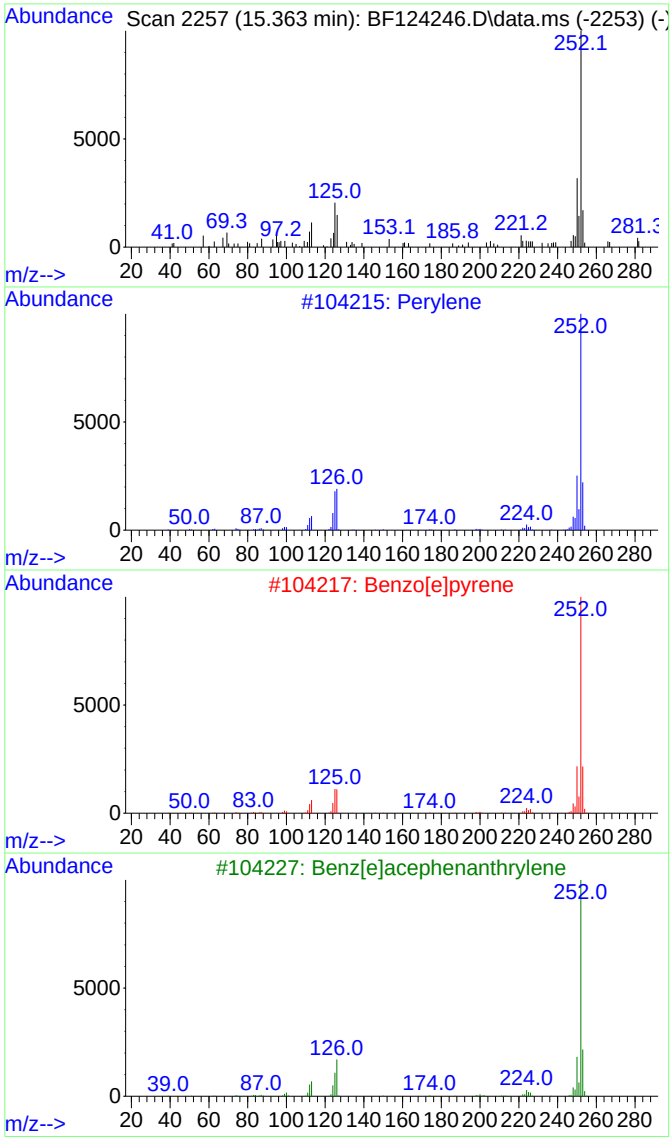
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

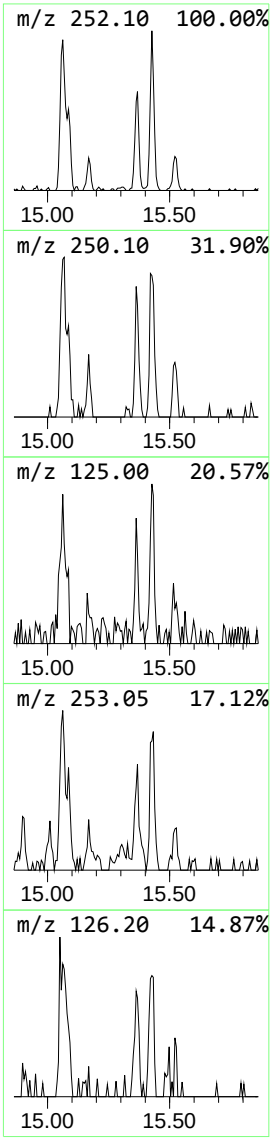
****

Peak Number 8 Perylene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.363	5.08 ng	79730	Perylene-d12	15.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	94
2	Benzo[e]pyrene	252	C20H12	000192-97-2	94
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	94
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061021\
Data File : BF124246.D
Acq On : 10 Jun 2021 22:33
Operator : JU/CG
Sample : M2651-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 17-B6(0-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
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
unknown5.057	5.057	3.3	ng	37778	1	6.845	227205	20.0
unknown6.681	6.681	3.9	ng	43721	1	6.845	227205	20.0
Benzenemethanet...	7.698	2.1	ng	30500	2	8.128	295050	20.0
Benzene, (1-bro...	9.334	5.8	ng	101947	3	9.886	351679	20.0
unknown11.898	11.898	3.7	ng	67082	4	11.375	361566	20.0
unknown13.857	13.857	4.6	ng	97150	5	14.016	421487	20.0
Perylene	15.363	5.1	ng	79730	6	15.492	313785	20.0