LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110430.D
Acq On : 2 Nov 2018 23:42
Operator : JU/SJ
Sample : J5769-05 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WAGARAW-RD-3

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-BF102318.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	2.263	25	30	43	rVB	157308	225884	21.79%	1.920%
2	5.181	523	526	531	rBV	34074	37060	3.57%	0.315%
3	5.575	589	593	605	rVB	926462	897780	86.59%	7.632%
4	6.510	749	752	758	rBV	43851	42603	4.11%	0.362%
5	6.575	759	763	777	rVB	940036	998757	96.33%	8.490%
6	6.722	784	788	792	rBV	1164994	977527	94.29%	8.310%
7	6.775	795	797	801	rVB	25551	20742	2.00%	0.176%
8	6.951	824	827	833	rBV	580460	551461	53.19%	4.688%
9	7.110	850	854	864	rVB	906716	766256	73.91%	6.514%
10	7.516	919	923	931	rBV	584006	579921	55.94%	4.930%
11	8.204	1036	1040	1042	rBV	12232	11449	1.10%	0.097%
12	8.239	1042	1046	1064	rVB	691452	701244	67.64%	5.961%
13	8.639	1110	1114	1117	rBV	19668	16269	1.57%	0.138%
14	8.810	1140	1143	1147	rVB	18367	14807	1.43%	0.126%
15	8.957	1164	1168	1173	rBV	15811	17754	1.71%	0.151%
16	9.051	1181	1184	1187	rBV	19062	16927	1.63%	0.144%
17	9.310	1224	1228	1237	rBV	1171039	1036772	100.00%	8.813%
18	9.374	1237	1239	1243	rVB	21394	20206	1.95%	0.172%
19	9.580	1270	1274	1279	rBV	7588	12598	1.22%	0.107%
20	9.651	1283	1286	1289	rVV	18672	19174	1.85%	0.163%
21	9.704	1292	1295	1302	rVB	116313	128687	12.41%	1.094%
22	9.857	1318	1321	1325	rBV	27283	24893	2.40%	0.212%
23	9.904	1325	1329	1332	rVV2	19991	19633	1.89%	0.167%
24	9.998	1341	1345	1353	rVB	696616	641911	61.91%	5.457%
25	10.404	1410	1414	1419	rBV2	31757	31559	3.04%	0.268%
26	10.539	1435	1437	1445	rVB4	8912	16022	1.55%	0.136%
27	10.627	1445	1452	1454	rBV2	11642	15545	1.50%	0.132%
28	10.786	1475	1479	1490	rVB	488285	462819	44.64%	3.934%
29	10.892	1492	1497	1500	rBV3	30362	41392	3.99%	0.352%
30	11.221	1548	1553	1555	rBV4	10063	12402	1.20%	0.105%
31	11.292	1562	1565	1569	rBV2	9106	12079	1.17%	0.103%
32	11.327	1569	1571	1574	rBV2	22438	19273	1.86%	0.164%
33	11.486	1594	1598	1601	rBV	570000	546806	52.74%	4.648%
34	11.510	1601	1602	1608	rVV	117552	92994	8.97%	0.791%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110430.D
Acq On : 2 Nov 2018 23:42
Operator : JU/SJ
Sample : J5769-05 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WAGARAW-RD-3

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-BF102318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.568	1608	1612	1615	rVV	15930	16038	1.55%	0.136%
36	11.757	1641	1644	1646	rVB2	18285	15787	1.52%	0.134%
37	11.992	1681	1684	1686	rBV	73559	68658	6.62%	0.584%
38	12.015	1686	1688	1694	rVB2	40424	48377	4.67%	0.411%
39	12.104	1699	1703	1705	rVV2	31600	39613	3.82%	0.337%
40	12.121	1705	1706	1710	rVB	22633	20385	1.97%	0.173%
41	12.163	1710	1713	1716	rBV2	17568	17189	1.66%	0.146%
42	12.286	1729	1734	1737	rBV2	21657	25230	2.43%	0.214%
43	12.315	1737	1739	1744	rVB2	18557	21056	2.03%	0.179%
44	12.433	1754	1759	1762	rBV6	9367	15062	1.45%	0.128%
45	12.539	1773	1777	1780	rBV2	34959	44672	4.31%	0.380%
46	12.627	1789	1792	1796	rBV4	22235	28183	2.72%	0.240%
47	12.704	1802	1805	1809	rBV	184870	160385	15.47%	1.363%
48	12.774	1814	1817	1819	rBV3	10424	15439	1.49%	0.131%
49	12.933	1838	1844	1850	rBV	165887	202198	19.50%	1.719%
50	12.986	1850	1853	1856	rVB2	21388	22548	2.17%	0.192%
51	13.068	1863	1867	1870	rBV	868692	754514	72.78%	6.414%
52	13.145	1877	1880	1885	rBV4	20574	38368	3.70%	0.326%
53	13.245	1893	1897	1898	rBV4	21027	26196	2.53%	0.223%
54	13.262	1898	1900	1901	rVV	18533	14124	1.36%	0.120%
55	13.327	1909	1911	1913	rBV2	16826	11364	1.10%	0.097%
56	13.368	1915	1918	1921	rVV2	20368	22483	2.17%	0.191%
57	13.462	1932	1934	1936	rBV	16788	12380	1.19%	0.105%
58	13.621	1958	1961	1962	rBV	19276	19401	1.87%	0.165%
59	13.739	1979	1981	1984	rBV4	17723	19897	1.92%	0.169%
60	13.774	1984	1987	1991	rVB	28071	33651	3.25%	0.286%
61	13.951	2013	2017	2020	rBV2	87845	107454	10.36%	0.913%
62	14.133	2044	2048	2051	rBV2	499461	525941	50.73%	4.471%
63	14.162	2051	2053	2055	rVB	68795	56596	5.46%	0.481%
64	15.204	2228	2230	2233	rBV	43824	51803	5.00%	0.440%
65	15.662	2304	2308	2312	rVB	208433	277726	26.79%	2.361%

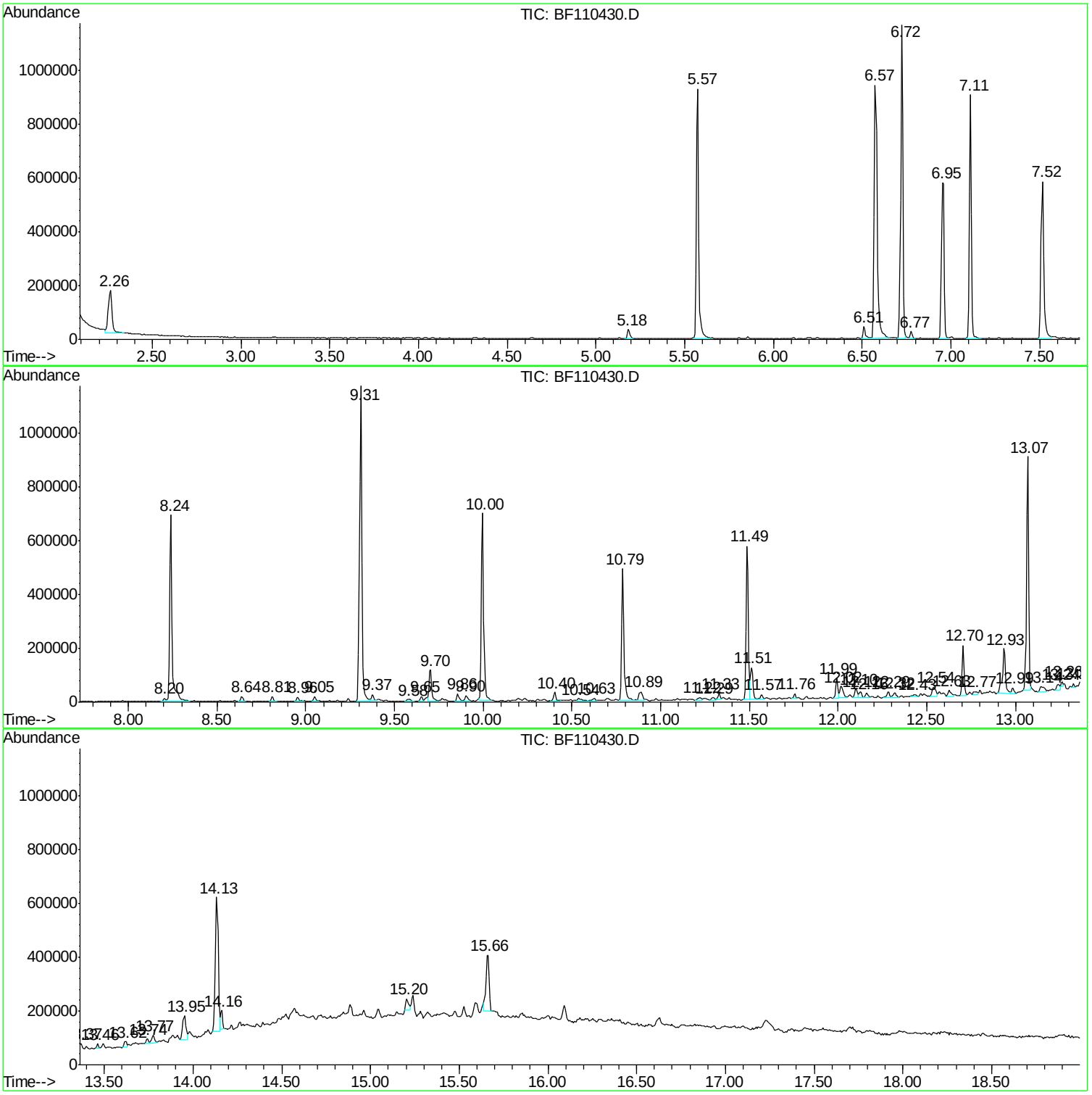
Sum of corrected areas: 11763924

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110430.D
Acq On : 2 Nov 2018 23:42
Operator : JU/SJ
Sample : J5769-05 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WAGARAW-RD-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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\BF110218\
Data File : BF110430.D
Acq On : 2 Nov 2018 23:42
Operator : JU/SJ
Sample : J5769-05 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WAGARAW-RD-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

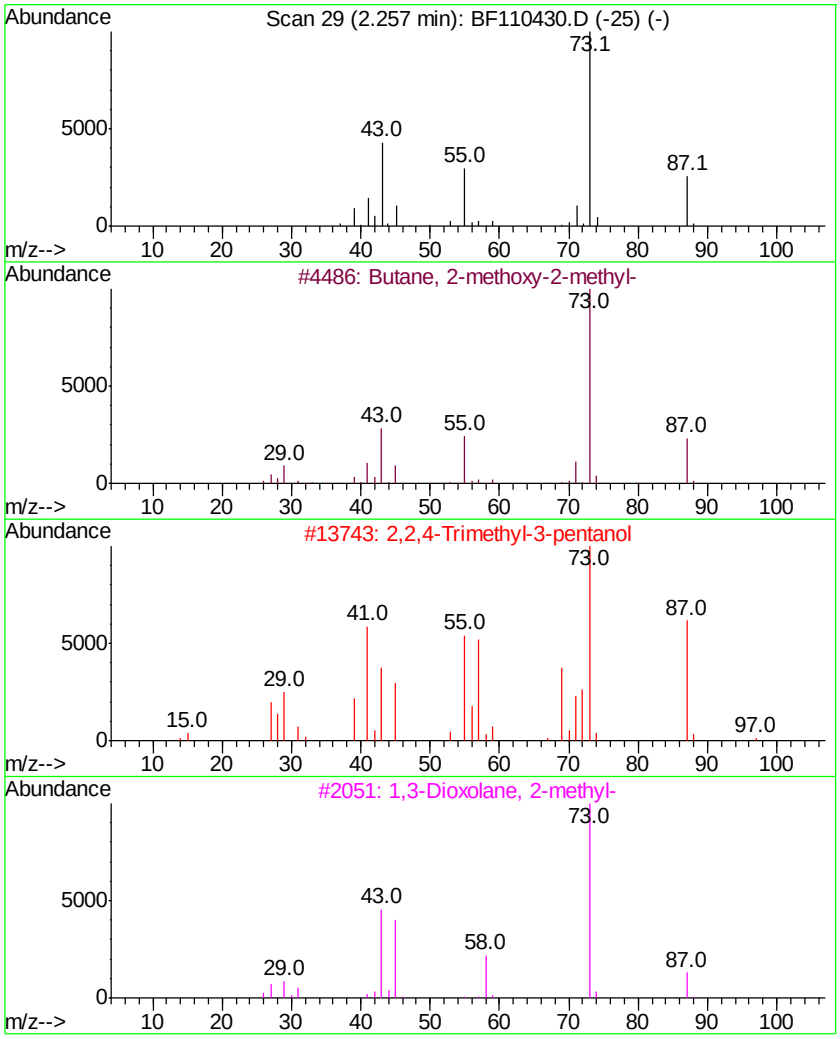
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

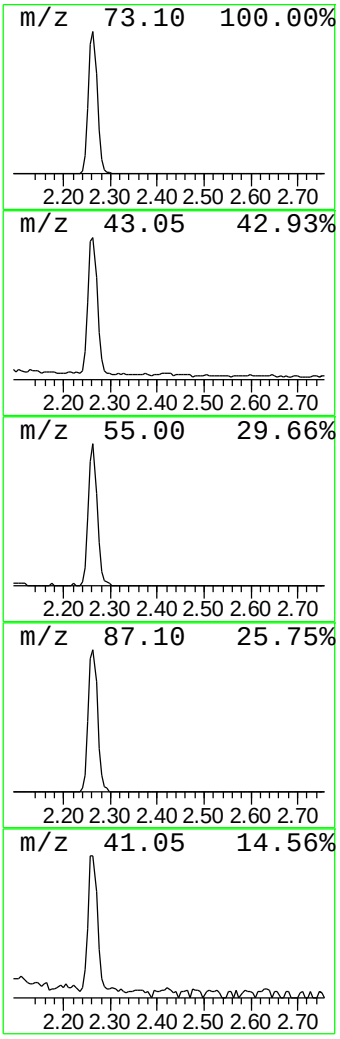
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.26	8.19 ng	225884	1,4-Dichlorobenzene-d4	6.96

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	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110430.D
Acq On : 2 Nov 2018 23:42
Operator : JU/SJ
Sample : J5769-05 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WAGARAW-RD-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

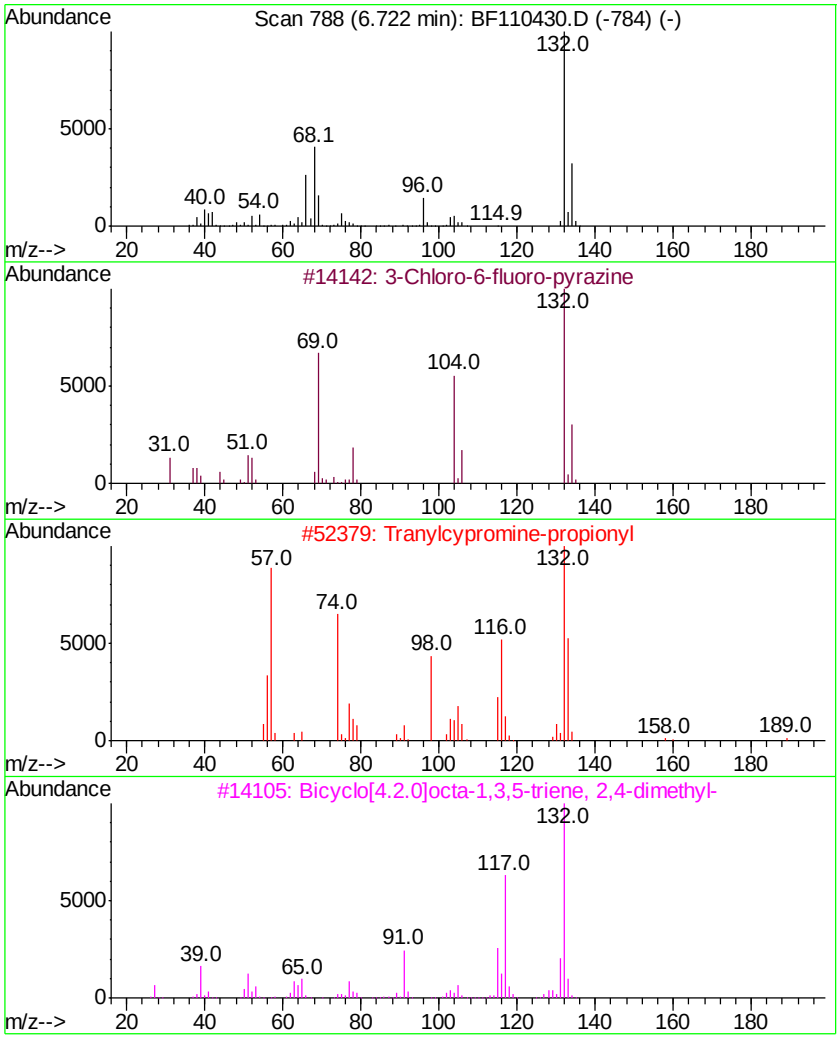
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

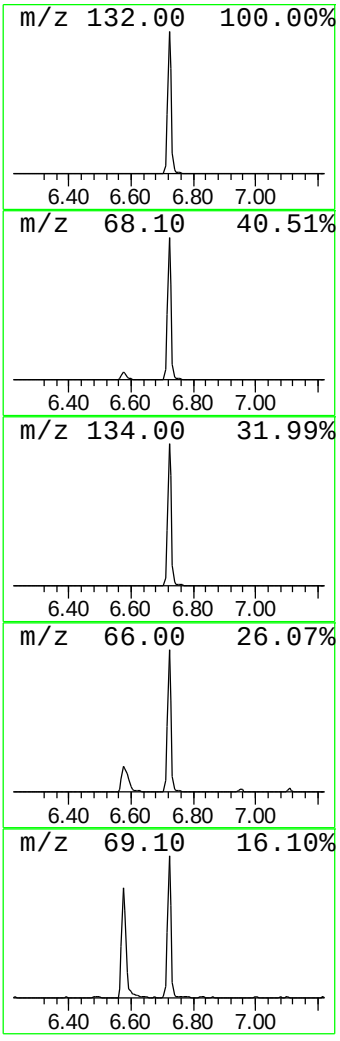
****

Peak Number 2 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	35.45 ng	977527	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110430.D
Acq On : 2 Nov 2018 23:42
Operator : JU/SJ
Sample : J5769-05 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WAGARAW-RD-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

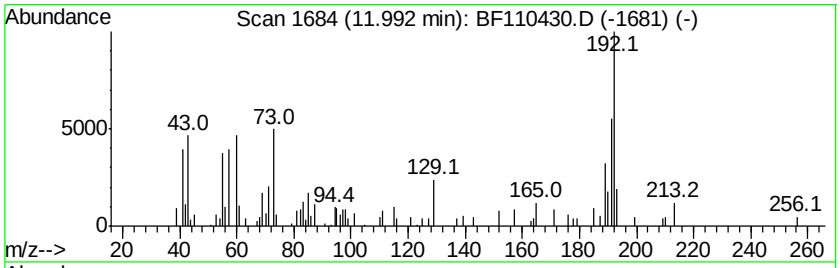
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

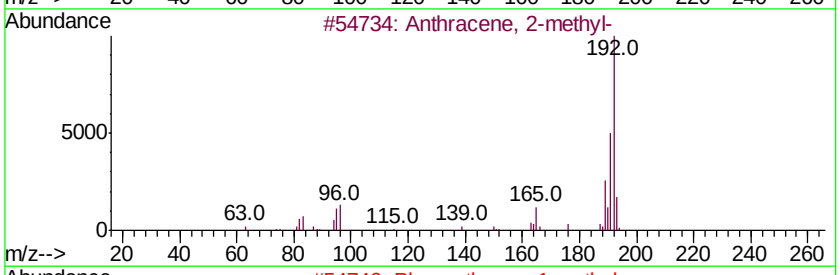
****

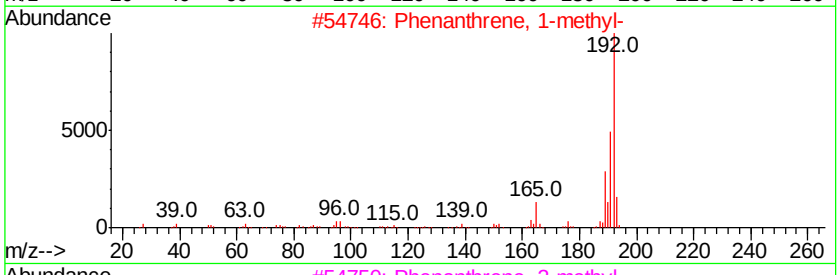
Peak Number 4 Anthracene, 2-methyl- Concentration Rank 5

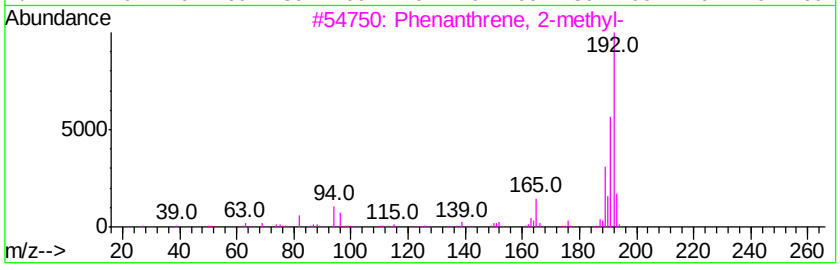
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	2.51 ng	68658	Phenanthrene-d10	11.49

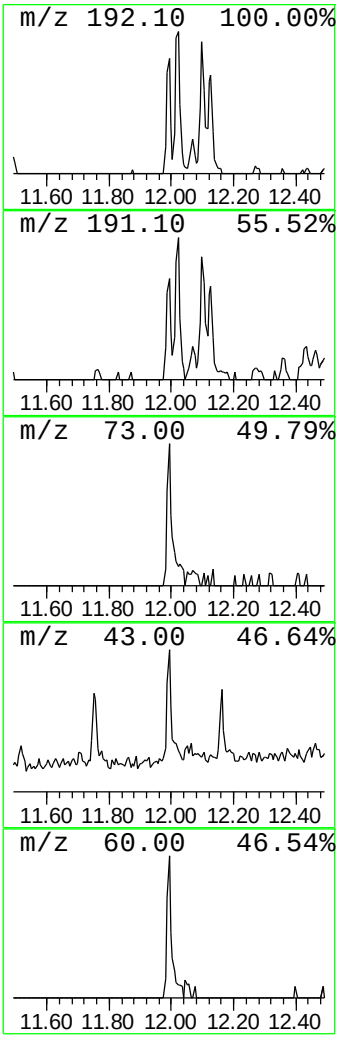
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	58
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	55
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	49
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	49
5	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	49











Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110430.D
Acq On : 2 Nov 2018 23:42
Operator : JU/SJ
Sample : J5769-05 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WAGARAW-RD-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

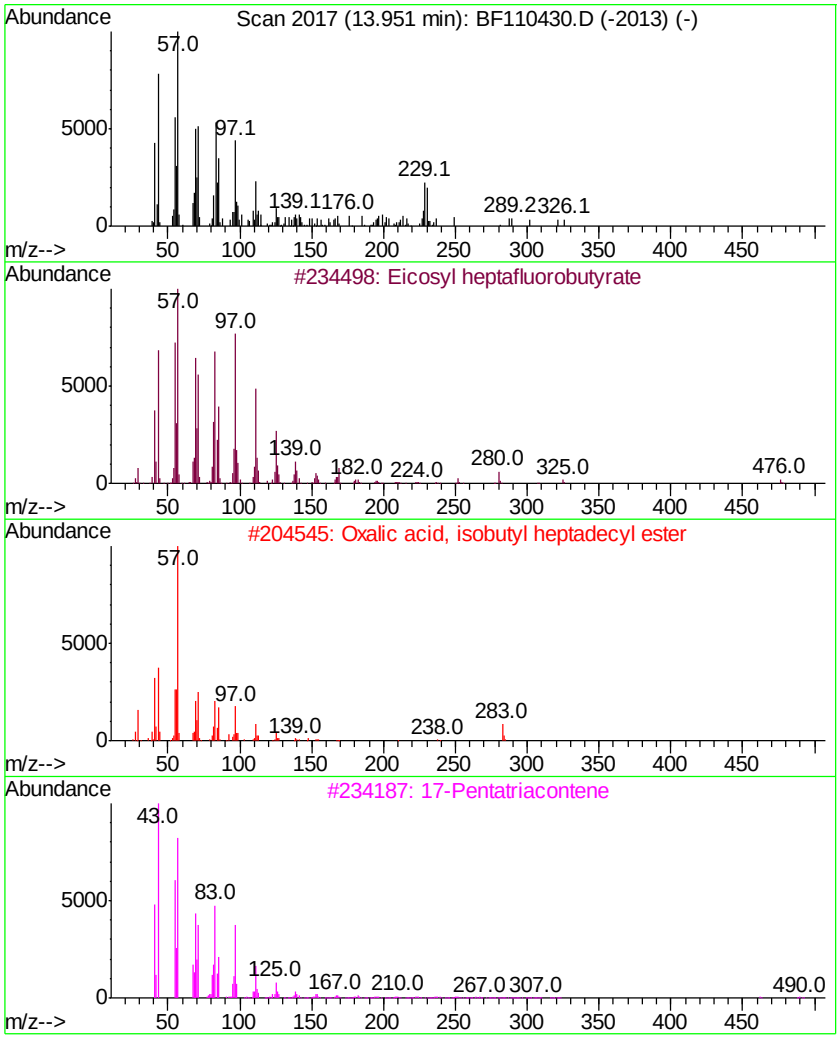
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

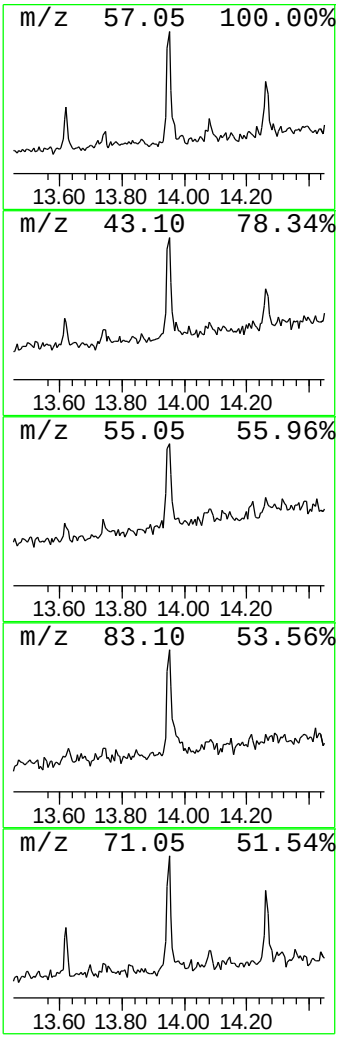
****

Peak Number 5 Eicosyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	4.09 ng	107454	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	64
2	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	62
3	17-Pentatriacontene	491	C35H70	006971-40-0	62
4	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	62
5	1,2-Octadecanediol	286	C18H38O2	020294-76-2	55





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110218\
Data File : BF110430.D
Acq On : 2 Nov 2018 23:42
Operator : JU/SJ
Sample : J5769-05 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WAGARAW-RD-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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
Butane, 2-methoxy...	2.26	8.2	ng	225884	1	6.96	551461	20.0
unknown6.72	6.72	35.5	ng	977527	1	6.96	551461	20.0
Anthracene, 2-met...	11.99	2.5	ng	68658	4	11.49	546806	20.0
Eicosyl heptafluo...	13.95	4.1	ng	107454	5	14.13	525941	20.0