LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091317\
Data File : BF098485.D
Acq On : 13 Sep 2017 13:01
Operator : SJ/JU
Sample : I5140-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-13-16-32

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:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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	3.575	247	253	263	rBV	446563	725582	14.44%	1.472%
2	4.846	465	469	483	rBV	303560	481943	9.59%	0.978%
3	5.269	536	541	555	rBV	4446514	4974525	99.00%	10.094%
4	6.304	712	717	728	rBV	4364232	5024666	100.00%	10.196%
5	6.428	733	738	741	rBV	5038386	4679493	93.13%	9.495%
6	6.651	773	776	782	rBV	1320395	1130165	22.49%	2.293%
7	6.810	799	803	806	rBV	3621822	3308457	65.84%	6.713%
8	7.081	846	849	858	rVB	281199	313099	6.23%	0.635%
9	7.222	868	873	876	rBV	3052082	2869408	57.11%	5.822%
10	7.710	945	956	960	rBV	209223	277832	5.53%	0.564%
11	7.934	990	994	997	rBV	1607909	1621824	32.28%	3.291%
12	7.957	997	998	1004	rVB	406406	269528	5.36%	0.547%
13	8.587	1099	1105	1110	rBV2	40200	61780	1.23%	0.125%
14	8.645	1112	1115	1119	rVB	113242	98870	1.97%	0.201%
15	8.745	1124	1132	1136	rVB	86068	85097	1.69%	0.173%
16	8.869	1149	1153	1160	rBV	107488	120888	2.41%	0.245%
17	9.010	1172	1177	1181	rBV	3992566	3867482	76.97%	7.848%
18	9.281	1218	1223	1226	rBV3	33673	53635	1.07%	0.109%
19	9.345	1230	1234	1237	rBV2	62485	66074	1.31%	0.134%
20	9.410	1241	1245	1248	rVB	575248	468164	9.32%	0.950%
21	9.545	1263	1268	1273	rVB	104014	101509	2.02%	0.206%
22	9.622	1277	1281	1285	rVB2	60243	57409	1.14%	0.116%
23	9.686	1285	1292	1295	rBV	1774233	1616453	32.17%	3.280%
24	9.892	1323	1327	1328	rBV	72157	76252	1.52%	0.155%
25	10.122	1363	1366	1371	rBV2	80246	68333	1.36%	0.139%
26	10.228	1381	1384	1390	rBV	92982	95763	1.91%	0.194%
27	10.339	1397	1403	1406	rBV	61327	71242	1.42%	0.145%
28	10.475	1420	1426	1436	rBV	2713380	2642005	52.58%	5.361%
29	10.592	1443	1446	1454	rVB	128591	194540	3.87%	0.395%
30	10.781	1474	1478	1480	rBV2	40167	51639	1.03%	0.105%
31	10.975	1508	1511	1516	rBV	70443	68804	1.37%	0.140%
32	11.063	1524	1526	1531	rVB2	86918	92969	1.85%	0.189%
33	11.169	1539	1544	1546	rBV	1773019	1745851	34.75%	3.543%
34	11.186	1546	1547	1551	rVV	864949	680306	13.54%	1.380%

LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091317\
Data File : BF098485.D
Acq On : 13 Sep 2017 13:01
Operator : SJ/JU
Sample : I5140-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-13-16-32

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:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.239	1551	1556	1560	rVB	129093	154794	3.08%	0.314%
36	11.404	1581	1584	1590	rVB	89998	91431	1.82%	0.186%
37	11.663	1626	1628	1631	rBV	83969	78703	1.57%	0.160%
38	11.692	1631	1633	1637	rVB	118601	111361	2.22%	0.226%
39	11.745	1638	1642	1644	rBV2	52281	58906	1.17%	0.120%
40	11.775	1644	1647	1650	rBV	155730	156757	3.12%	0.318%
41	11.963	1676	1679	1681	rBV	75121	62658	1.25%	0.127%
42	11.992	1682	1684	1691	rVB	86863	95735	1.91%	0.194%
43	12.145	1707	1710	1712	rBV3	47688	56597	1.13%	0.115%
44	12.216	1719	1722	1724	rBV	87395	89597	1.78%	0.182%
45	12.304	1734	1737	1741	rBV4	59962	72330	1.44%	0.147%
46	12.375	1745	1749	1753	rVV	1024421	839367	16.70%	1.703%
47	12.469	1763	1765	1768	rBV	70197	63489	1.26%	0.129%
48	12.569	1779	1782	1783	rBV	114785	86505	1.72%	0.176%
49	12.604	1784	1788	1790	rVV	734058	724752	14.42%	1.471%
50	12.657	1794	1797	1801	rBV3	58747	57068	1.14%	0.116%
51	12.751	1808	1813	1816	rBV	3393797	3066803	61.03%	6.223%
52	12.775	1816	1817	1821	rVB	183443	147766	2.94%	0.300%
53	12.933	1841	1844	1847	rVB	137704	138581	2.76%	0.281%
54	12.998	1852	1855	1857	rVV	128842	119870	2.39%	0.243%
55	13.033	1859	1861	1868	rVB	112217	133994	2.67%	0.272%
56	13.292	1902	1905	1907	rBV	175845	155571	3.10%	0.316%
57	13.651	1963	1966	1972	rVB	314202	341176	6.79%	0.692%
58	13.798	1986	1991	1994	rBV2	1478901	1581793	31.48%	3.210%
59	13.822	1994	1995	2003	rVB	331274	238117	4.74%	0.483%
60	14.804	2159	2162	2169	rVB	212329	342370	6.81%	0.695%
61	14.904	2176	2179	2191	rVB	68416	127927	2.55%	0.260%
62	15.080	2206	2209	2215	rVB	128305	157105	3.13%	0.319%
63	15.139	2215	2219	2224	rVV	210172	253907	5.05%	0.515%
64	15.192	2224	2228	2240	rVB	805238	1112183	22.13%	2.257%
65	15.604	2295	2298	2302	rVB	71060	88769	1.77%	0.180%
66	16.057	2371	2375	2381	rVB2	62276	108736	2.16%	0.221%
67	16.527	2450	2455	2461	rBV4	91135	180923	3.60%	0.367%
68	16.927	2518	2523	2528	rBV	67033	125062	2.49%	0.254%

Sum of corrected areas: 49282290

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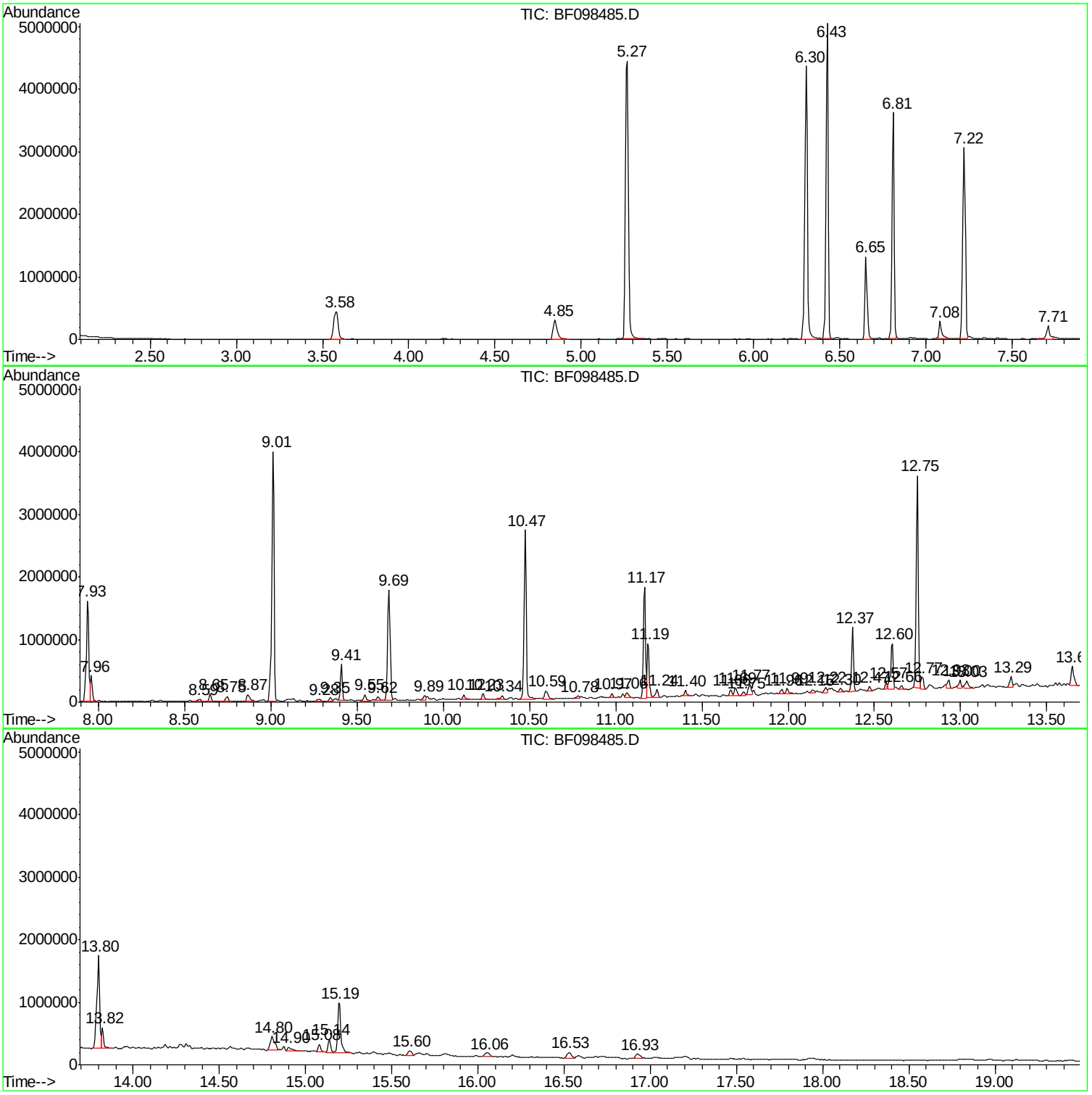
Acq On : 13 Sep 2017 13:01
Operator : SJ/JU
Sample : I5140-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RL-13-16-32

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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 : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091317\
Data File : BF098485.D
Acq On : 13 Sep 2017 13:01
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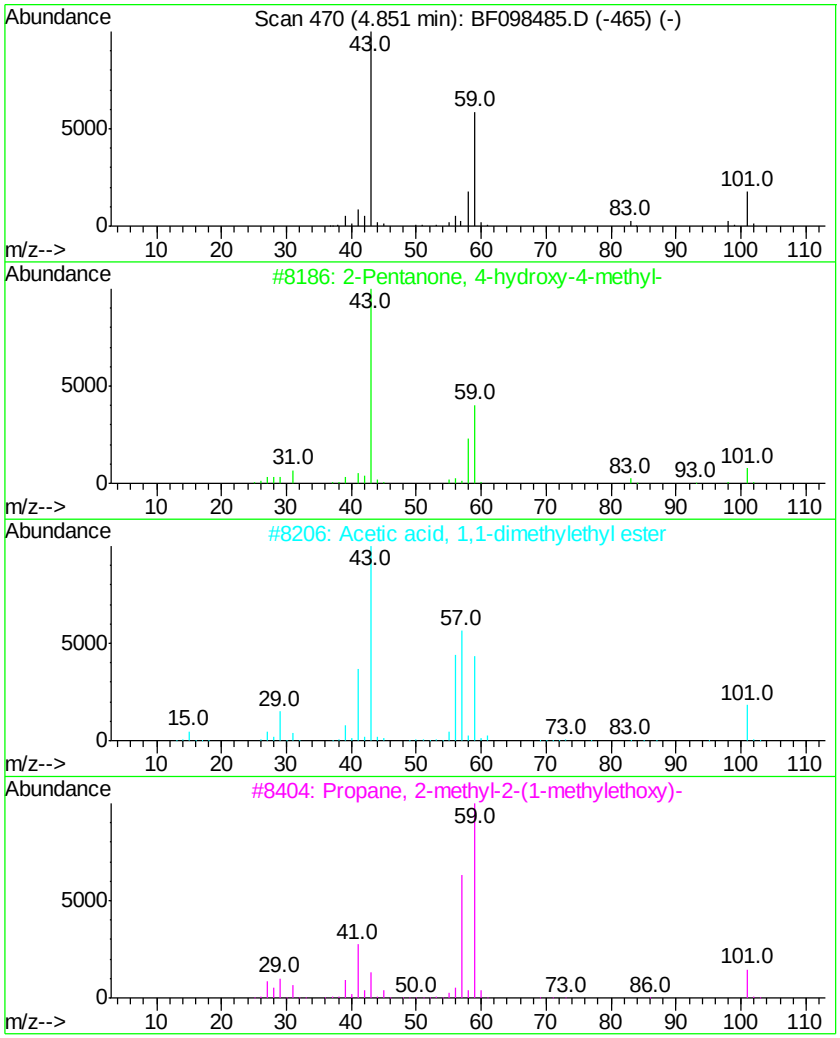
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

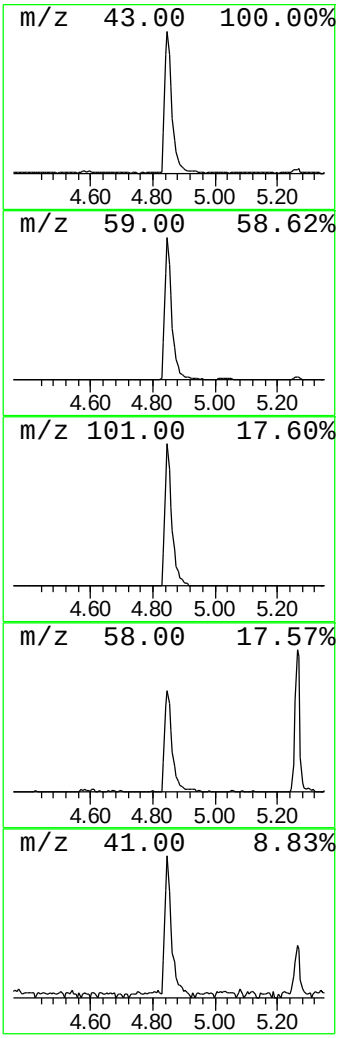
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	8.53 ng	481943	1,4-Dichlorobenzene-d4	6.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091317\
Data File : BF098485.D
Acq On : 13 Sep 2017 13:01
Operator : SJ/JU
Sample : I5140-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-13-16-32

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

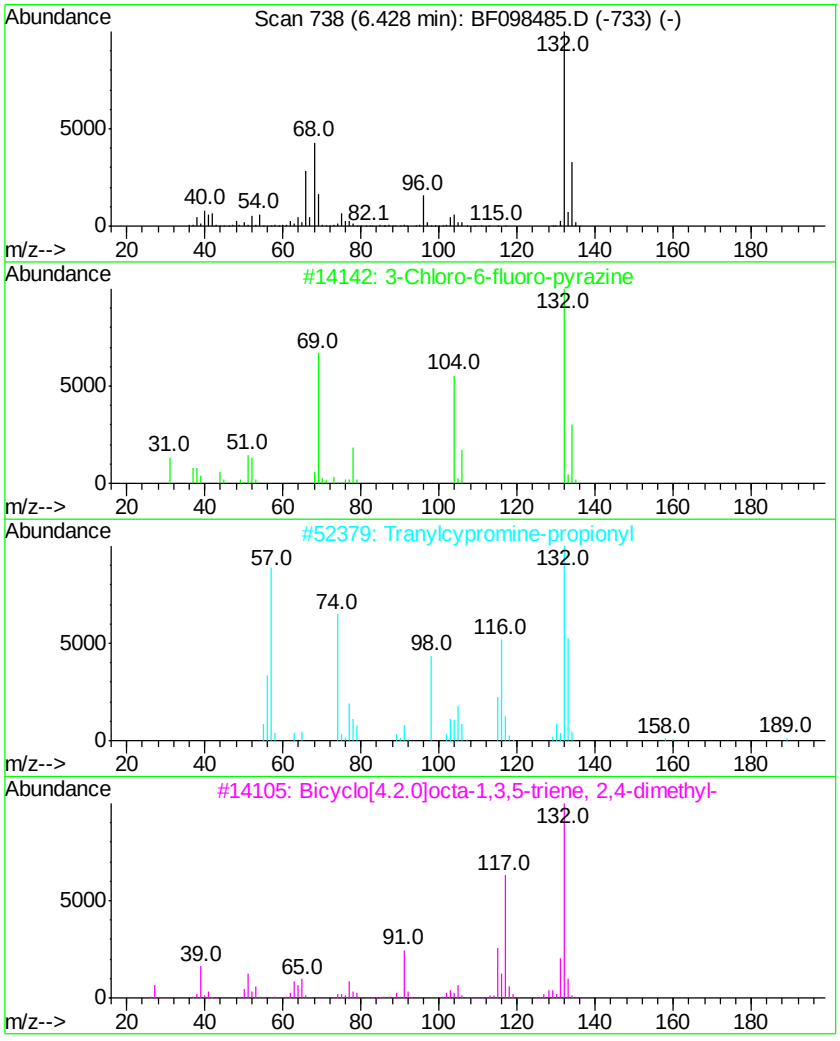
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

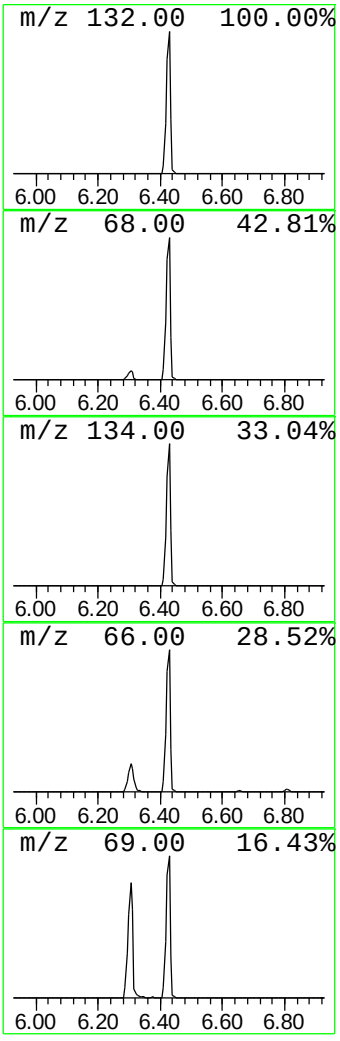
****

Peak Number 3 unknown6.43 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.43	82.81 ng	4679490	1,4-Dichlorobenzene-d4	6.65

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	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

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Data File : BF098485.D
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
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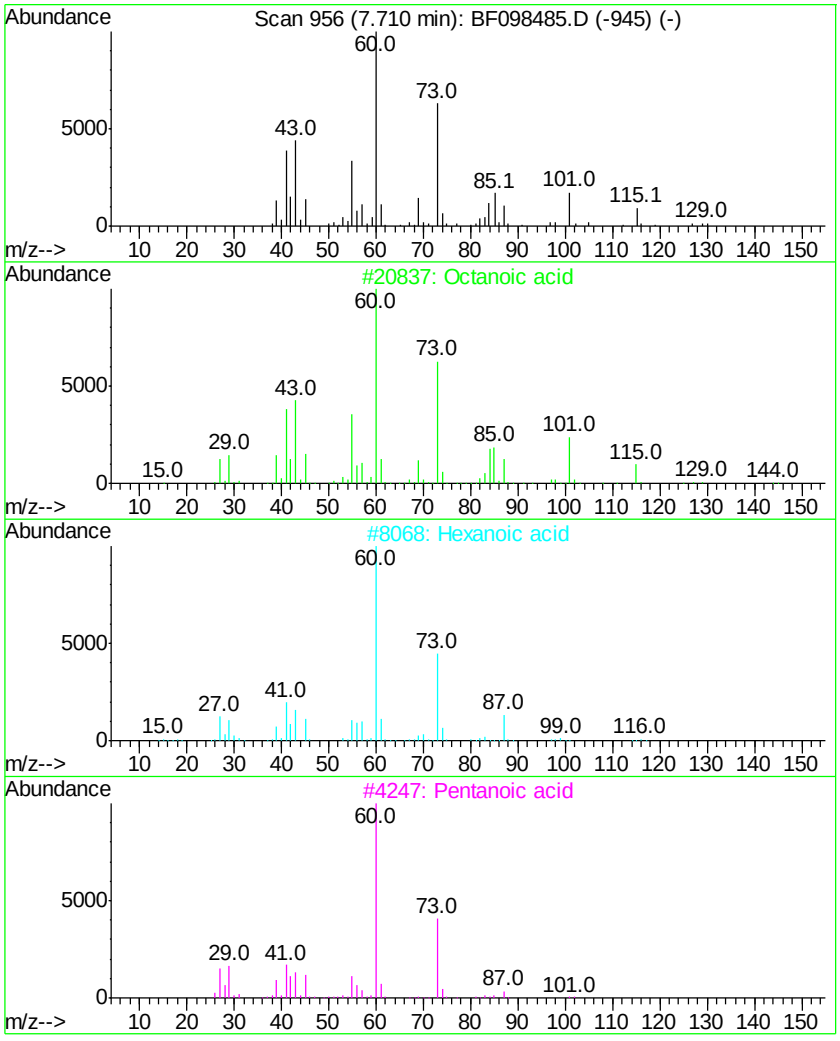
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

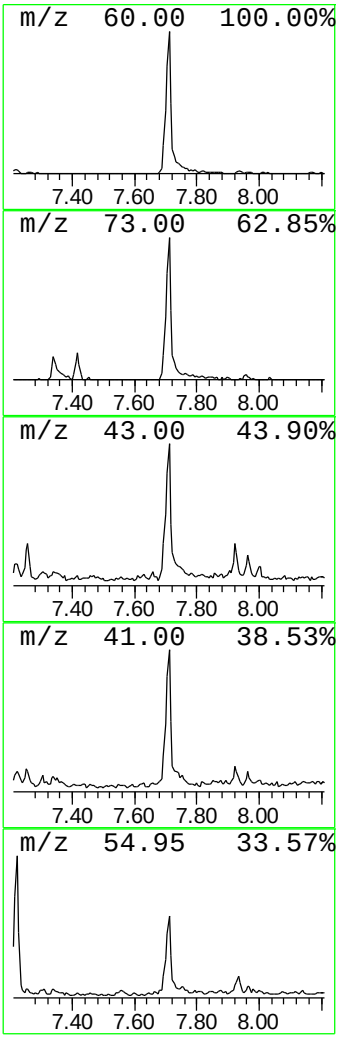
****

Peak Number 5 Octanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.71	3.43 ng	277832	Naphthalene-d8	7.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid	144	C8H16O2	000124-07-2	91
2	Hexanoic acid	116	C6H12O2	000142-62-1	64
3	Pentanoic acid	102	C5H10O2	000109-52-4	53
4	Heptanoic acid	130	C7H14O2	000111-14-8	53
5	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	42





Library Search Compound Report

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Data File : BF098485.D
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Sample : I5140-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-13-16-32

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

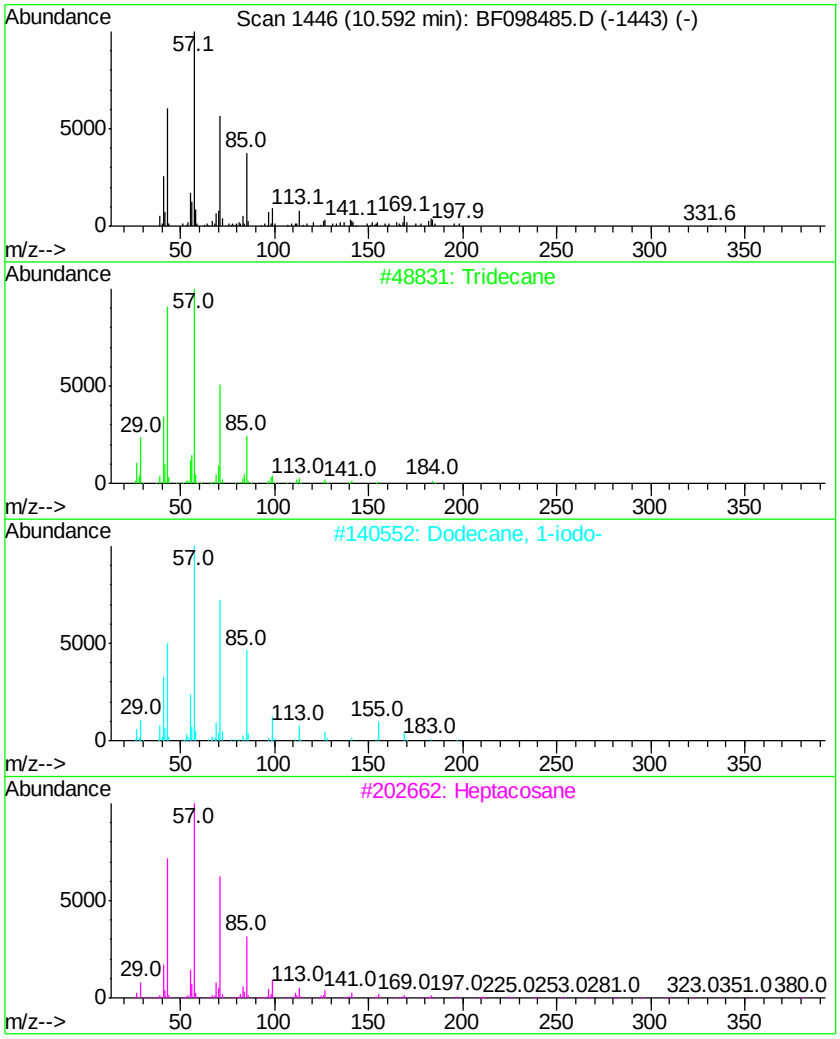
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

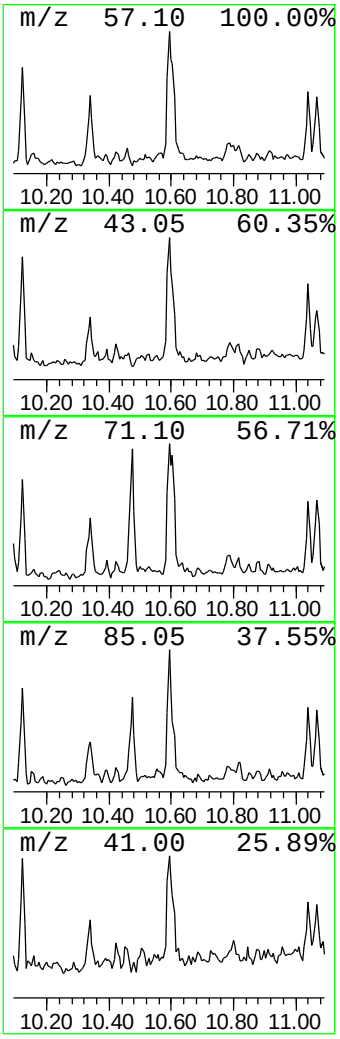
****

Peak Number 6 Tridecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.59	2.23 ng	194540	Phenanthrene-d10	11.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	83
2	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
3	Heptacosane	380	C27H56	000593-49-7	80
4	Dodecane	170	C12H26	000112-40-3	80
5	Hexadecane	226	C16H34	000544-76-3	72





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091317\
Data File : BF098485.D
Acq On : 13 Sep 2017 13:01
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Sample : I5140-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-13-16-32

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

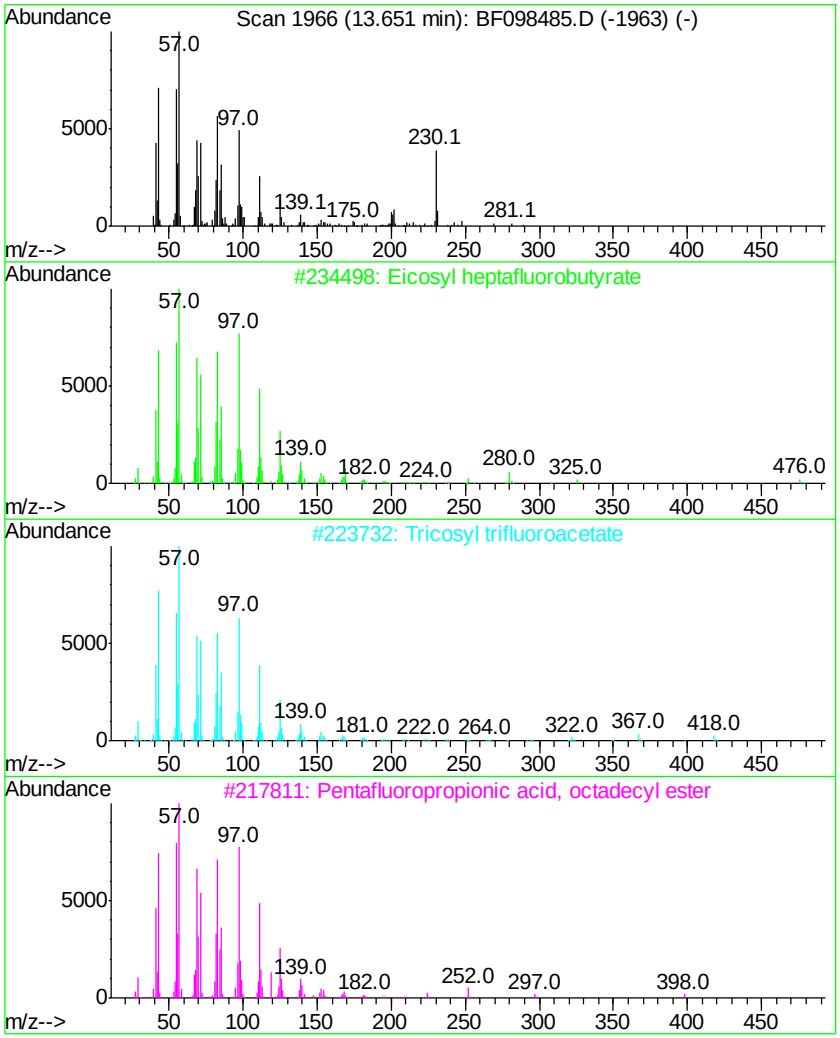
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

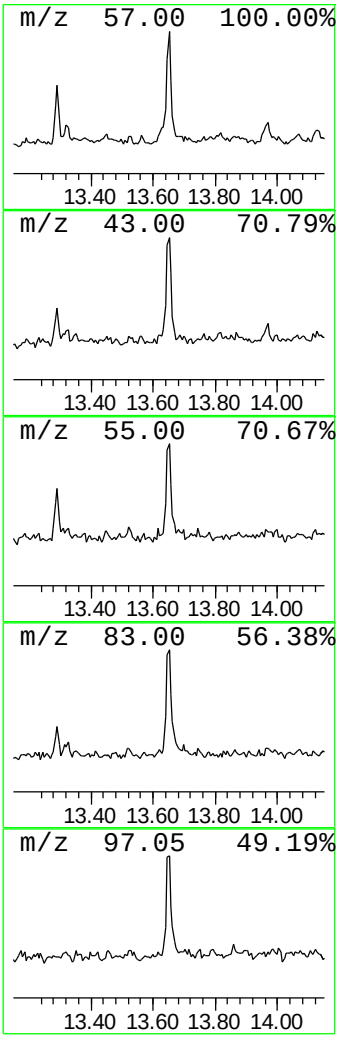
****

Peak Number 7 Eicosyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.65	4.31 ng	341176	Chrysene-d12	13.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	81
2	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	81
3	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	81
4	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	81
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	81





Library Search Compound Report

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Data File : BF098485.D
Acq On : 13 Sep 2017 13:01
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Sample : I5140-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-13-16-32

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

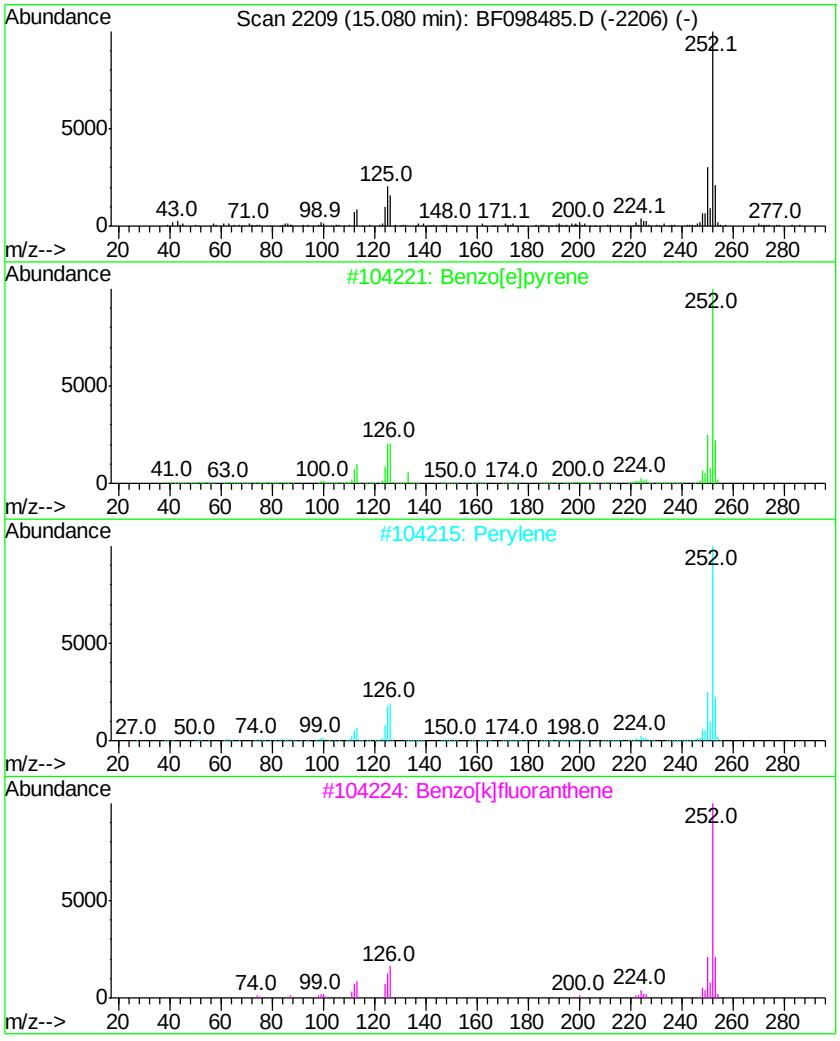
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

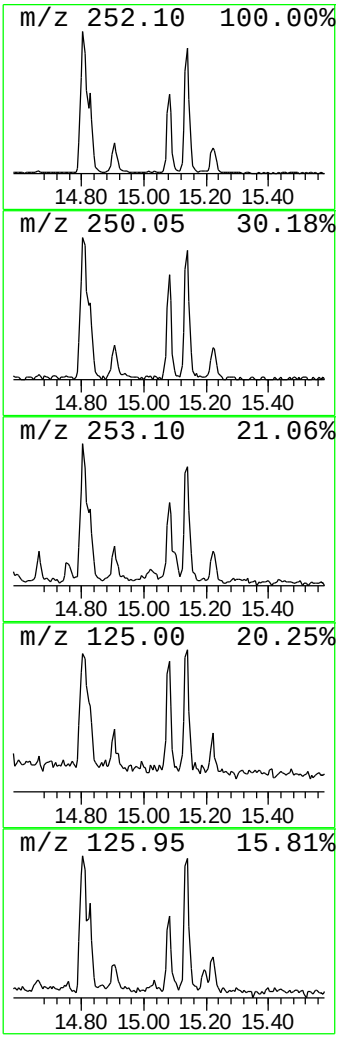
****

Peak Number 9 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.08	2.83 ng	157105	Perylene-d12	15.20

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	98
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
4	Benzo[a]pyrene	252	C20H12	000050-32-8	95
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF091317\
Data File : BF098485.D
Acq On : 13 Sep 2017 13:01
Operator : SJ/JU
Sample : I5140-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-13-16-32

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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
2-Pentanone, 4-hy...	4.85	8.5	ng	481943	1	6.65	1130170	20.0
unknown6.43	6.43	82.8	ng	4679490	1	6.65	1130170	20.0
Octanoic acid	7.71	3.4	ng	277832	2	7.93	1621820	20.0
Tridecane	10.59	2.2	ng	194540	4	11.17	1745850	20.0
Eicosyl heptafluo...	13.65	4.3	ng	341176	5	13.80	1581790	20.0
Benzo[e]pyrene	15.08	2.8	ng	157105	6	15.20	1112180	20.0