LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061118\
Data File : BF106311.D
Acq On : 11 Jun 2018 22:42
Operator : JU/SJ
Sample : J3347-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-11-12

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-BF061118.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	4.101	296	300	307	rVB	54127	67980	1.83%	0.178%
2	5.201	483	487	493	rVB	321167	350082	9.41%	0.914%
3	5.589	547	553	556	rBV	3770043	3612137	97.11%	9.435%
4	6.589	717	723	726	rBV	3631627	3719484	100.00%	9.716%
5	6.736	744	748	752	rBV	3626231	3663524	98.50%	9.569%
6	6.972	784	788	791	rVB	1595170	1209093	32.51%	3.158%
7	7.131	810	815	818	rBV	2962334	2759772	74.20%	7.209%
8	7.531	878	883	886	rBV	2633333	2329012	62.62%	6.084%
9	8.254	1002	1006	1009	rBV	1795216	1456105	39.15%	3.803%
10	9.325	1184	1188	1192	rBV	3879592	3642478	97.93%	9.514%
11	9.719	1252	1255	1258	rBV	519996	405746	10.91%	1.060%
12	9.930	1284	1291	1293	rVB	61949	59878	1.61%	0.156%
13	10.013	1301	1305	1308	rBV	1577741	1330094	35.76%	3.474%
14	10.195	1333	1336	1342	rBV3	52758	62876	1.69%	0.164%
15	10.430	1373	1376	1379	rVB	101389	82184	2.21%	0.215%
16	10.801	1435	1439	1442	rBV	2327204	2042015	54.90%	5.334%
17	10.901	1453	1456	1462	rBV2	94924	118257	3.18%	0.309%
18	11.001	1470	1473	1477	rBV3	44382	50818	1.37%	0.133%
19	11.036	1477	1479	1482	rVV2	48012	39797	1.07%	0.104%
20	11.089	1486	1488	1492	rBV3	49212	57438	1.54%	0.150%
21	11.148	1495	1498	1502	rVB3	48106	59036	1.59%	0.154%
22	11.189	1502	1505	1507	rBV	67000	55960	1.50%	0.146%
23	11.348	1529	1532	1535	rVB	53617	41224	1.11%	0.108%
24	11.501	1554	1558	1561	rBV	1531953	1228881	33.04%	3.210%
25	11.524	1561	1562	1566	rVB	113718	67853	1.82%	0.177%
26	11.707	1590	1593	1599	rBV2	91065	93639	2.52%	0.245%
27	12.013	1640	1645	1659	rBV2	718045	836600	22.49%	2.185%
28	12.113	1659	1662	1665	rBV2	45189	56438	1.52%	0.147%
29	12.524	1729	1732	1734	rBV	54887	44694	1.20%	0.117%
30	12.713	1760	1764	1770	rBV	239412	261876	7.04%	0.684%
31	12.801	1775	1779	1784	rBV	457091	428771	11.53%	1.120%
32	12.948	1798	1804	1806	rBV	220398	211225	5.68%	0.552%
33	13.089	1823	1828	1831	rBV	3504423	3449146	92.73%	9.009%
34	13.165	1837	1841	1847	rVB6	27454	49919	1.34%	0.130%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
ClientSampleId : B-11-12

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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Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.271	1857	1859	1862	rVB2	45375	43684	1.17%	0.114%
36	13.612	1914	1917	1920	rBV	161566	142731	3.84%	0.373%
37	13.777	1941	1945	1950	rVB2	47915	59816	1.61%	0.156%
38	13.965	1974	1977	1984	rVB2	579371	532001	14.30%	1.390%
39	14.148	2003	2008	2011	rBV	1630397	1555343	41.82%	4.063%
40	14.171	2011	2012	2018	rVB	136472	94076	2.53%	0.246%
41	14.295	2030	2033	2038	rBV4	42324	46007	1.24%	0.120%
42	14.536	2072	2074	2077	rVB	57166	47025	1.26%	0.123%
43	14.612	2083	2087	2093	rVB3	108724	136106	3.66%	0.356%
44	15.012	2152	2155	2161	rVB	80086	85565	2.30%	0.224%
45	15.218	2186	2190	2194	rBV	78987	135621	3.65%	0.354%
46	15.289	2199	2202	2204	rVB2	45166	47852	1.29%	0.125%
47	15.542	2243	2245	2251	rVB	60377	84258	2.27%	0.220%
48	15.606	2253	2256	2261	rVV	59110	92872	2.50%	0.243%
49	15.677	2263	2268	2280	rVB	865644	1123521	30.21%	2.935%
50	16.206	2355	2358	2365	rVB5	61574	113366	3.05%	0.296%

Sum of corrected areas: 38283876

LSC Report - Integrated Chromatogram

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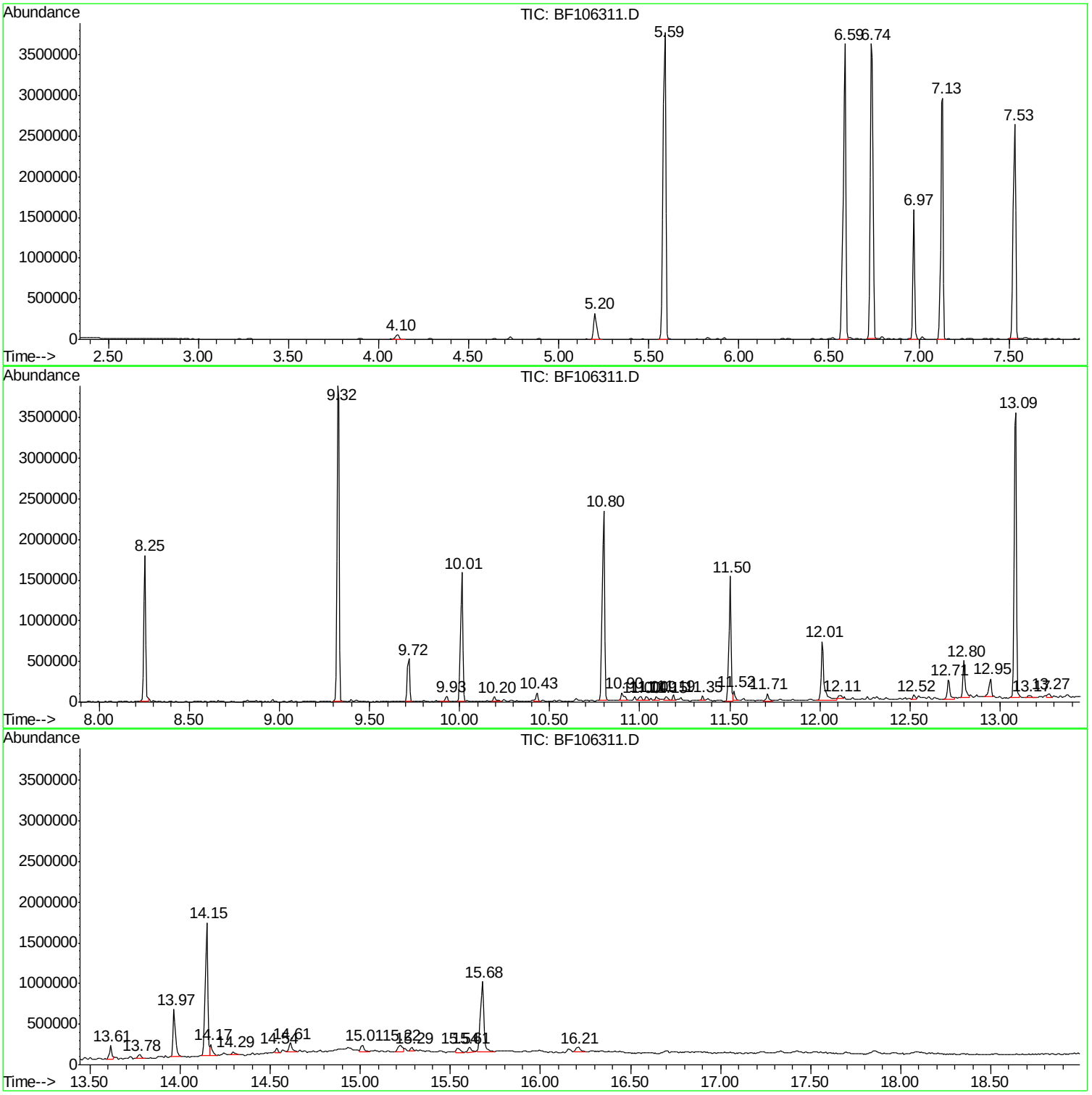
Sample : J3347-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-11-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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\BF061118\
Data File : BF106311.D
Acq On : 11 Jun 2018 22:42
Operator : JU/SJ
Sample : J3347-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-11-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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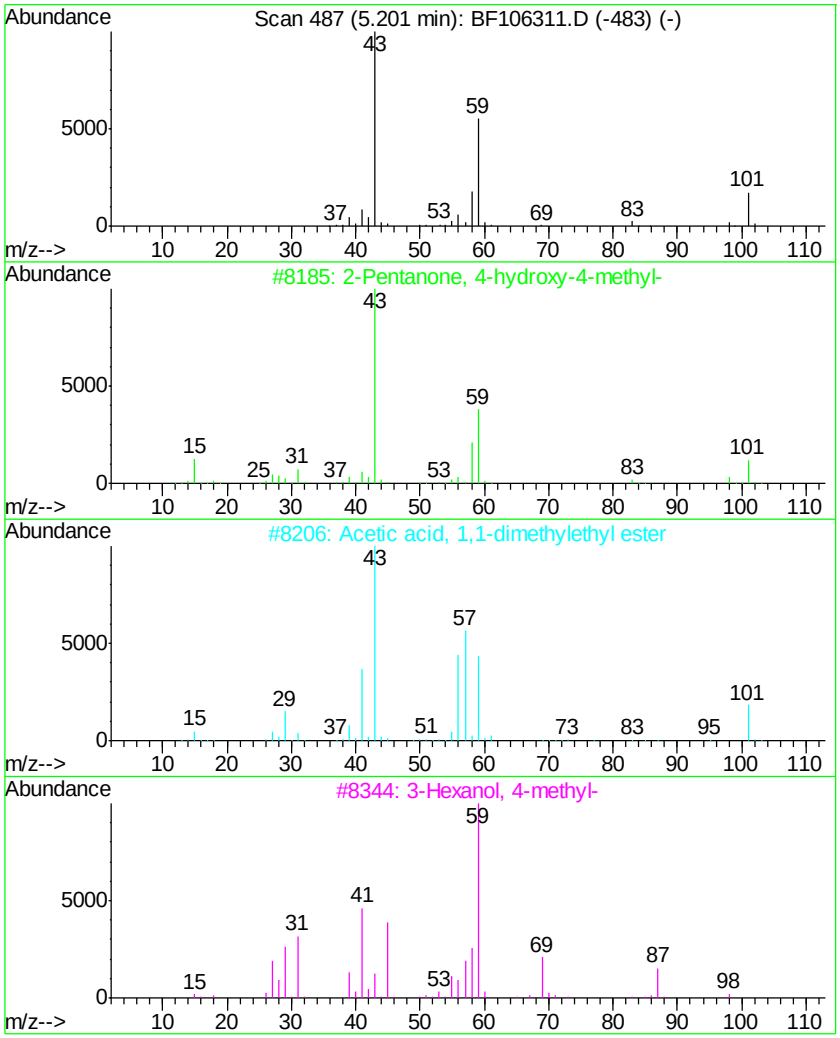
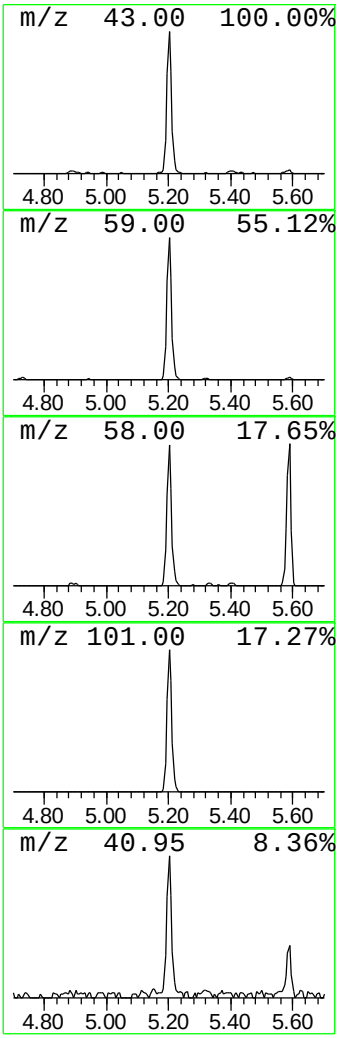
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	5.79 ng	350082	1,4-Dichlorobenzene-d4	6.97

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	38
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Library Search Compound Report

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Operator : JU/SJ
Sample : J3347-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-11-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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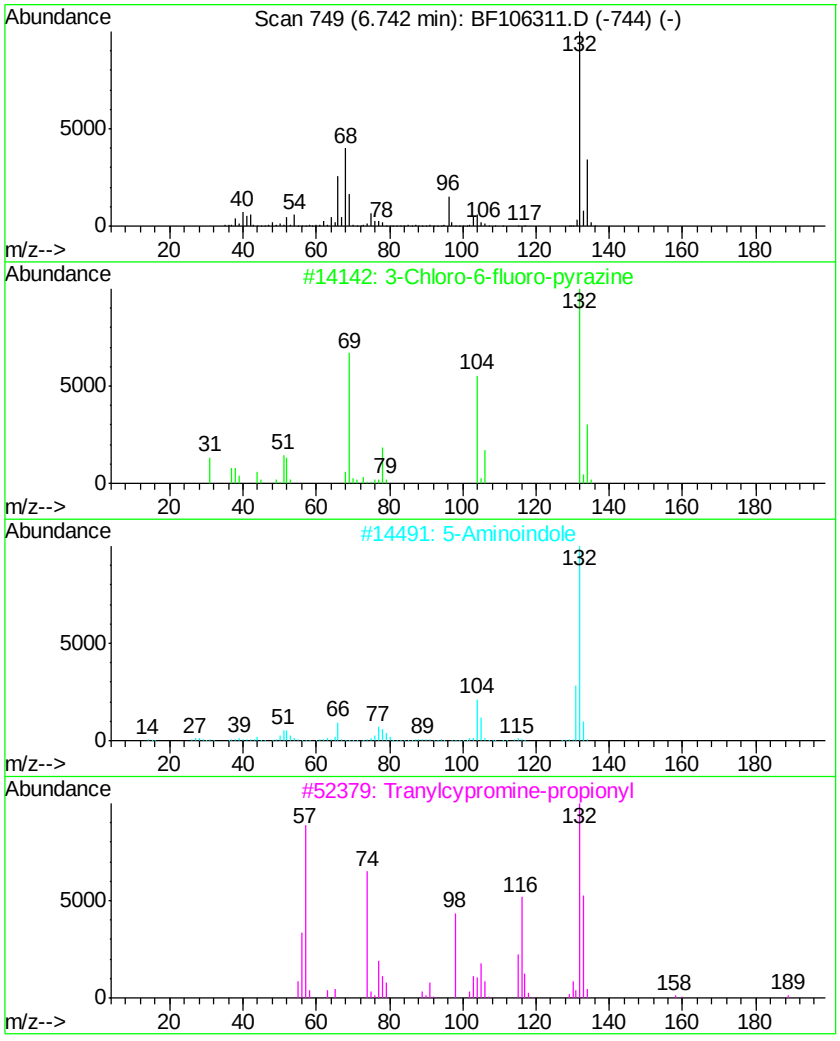
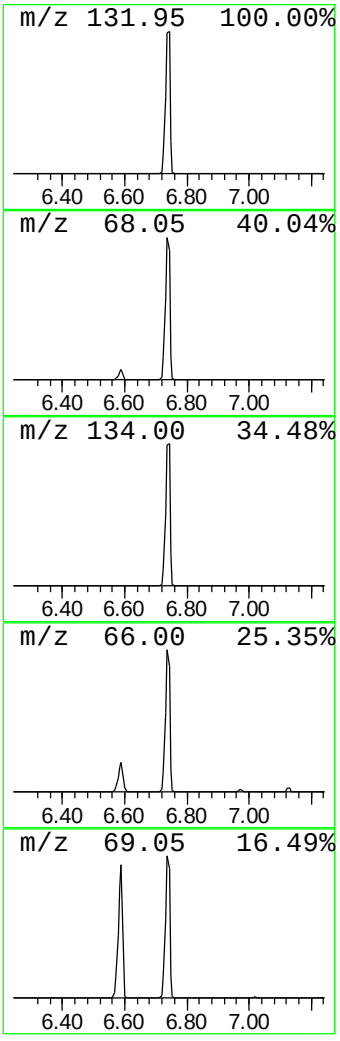
Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	60.60 ng	3663520	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Sample : J3347-01
Misc :
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Instrument : BNA_F
ClientSampleId : B-11-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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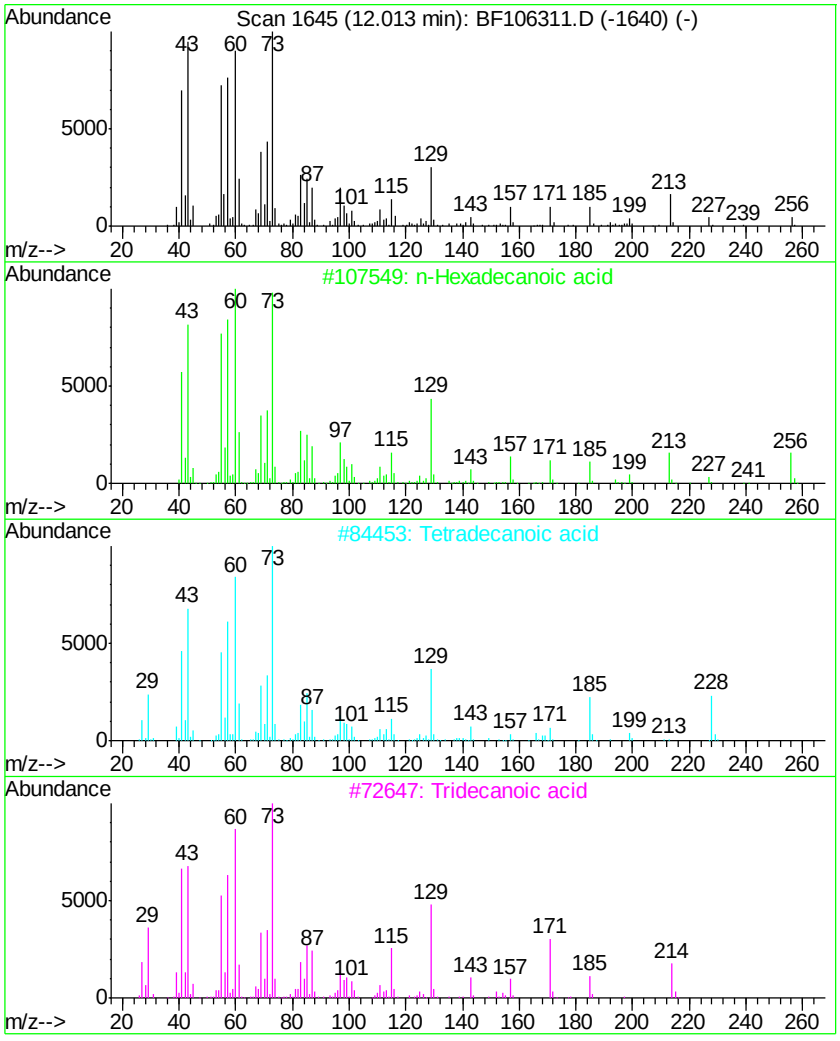
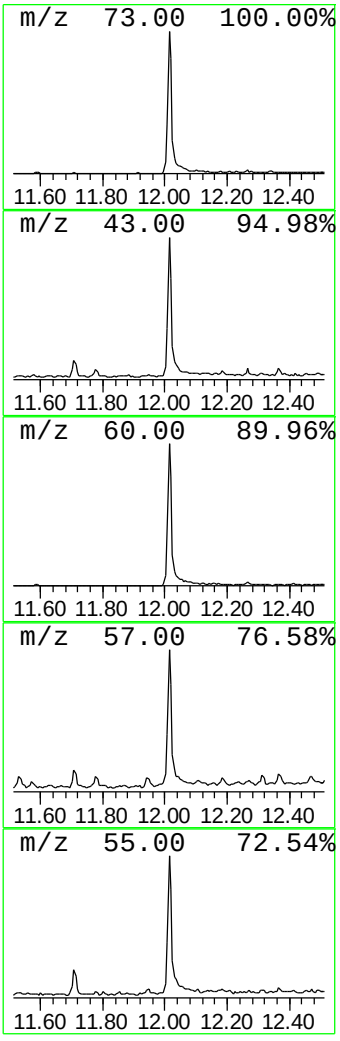
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	13.62 ng	836600	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3	Tridecanoic acid	214	C13H26O2	000638-53-9	95
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	n-Decanoic acid	172	C10H20O2	000334-48-5	25





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Misc :
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Instrument : BNA_F
ClientSampleId : B-11-12

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

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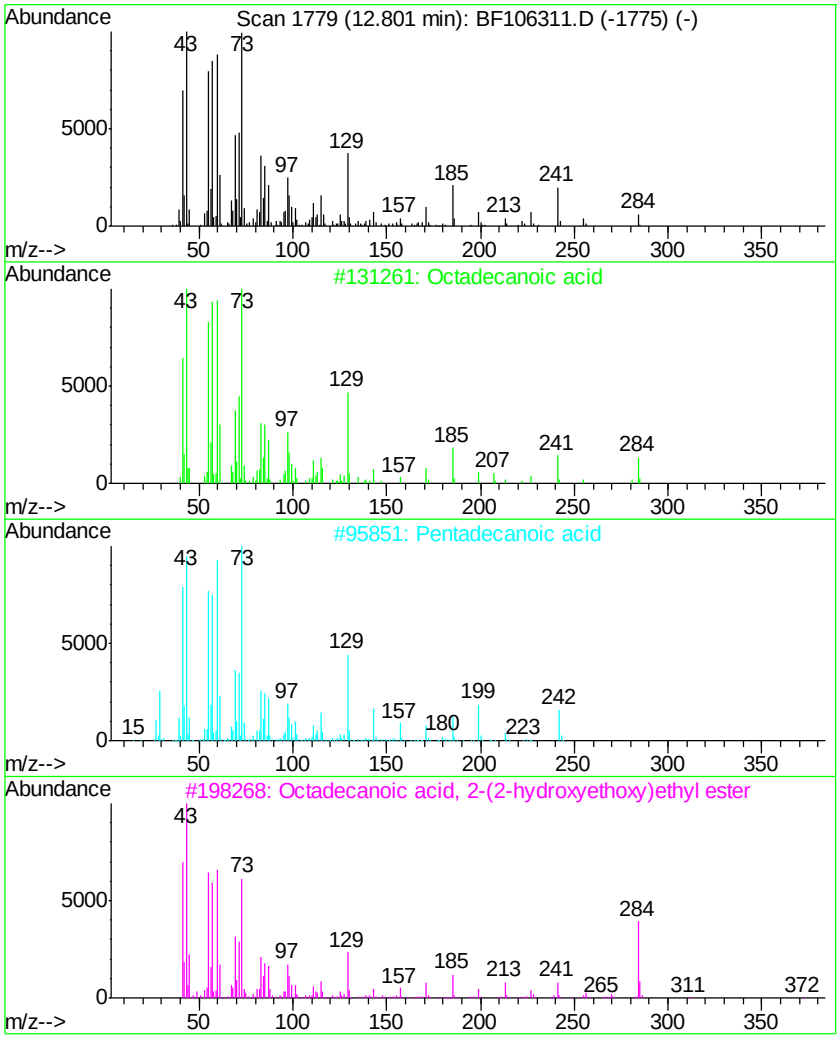
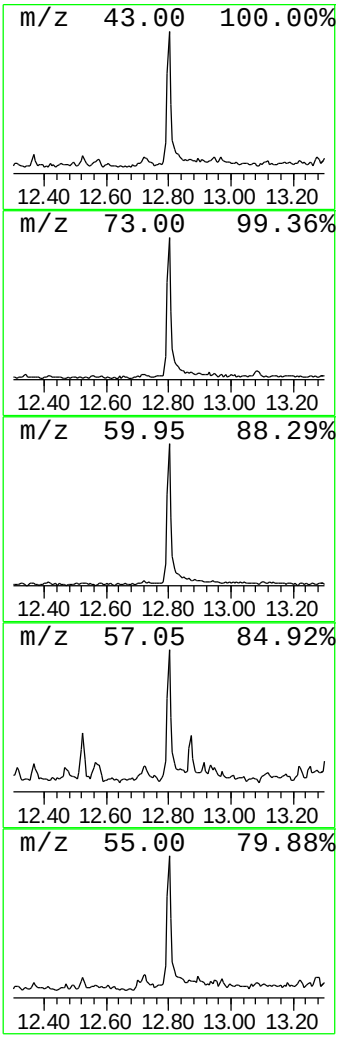
Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	6.98 ng	428771	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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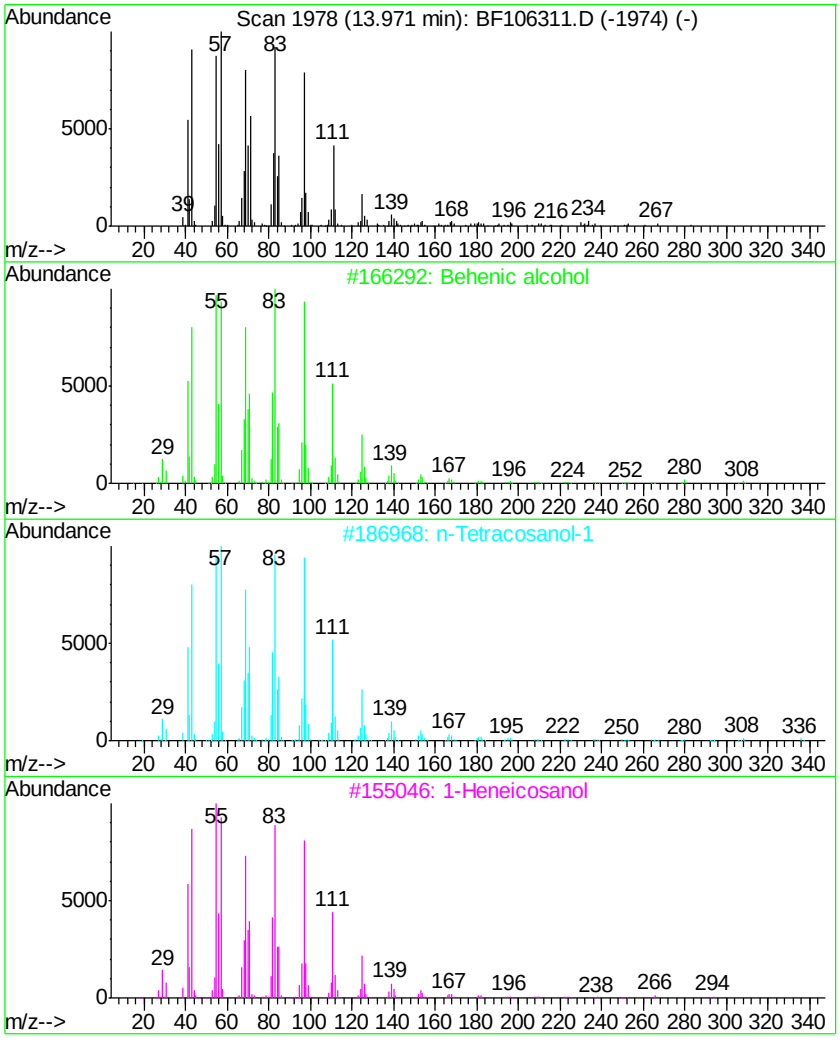
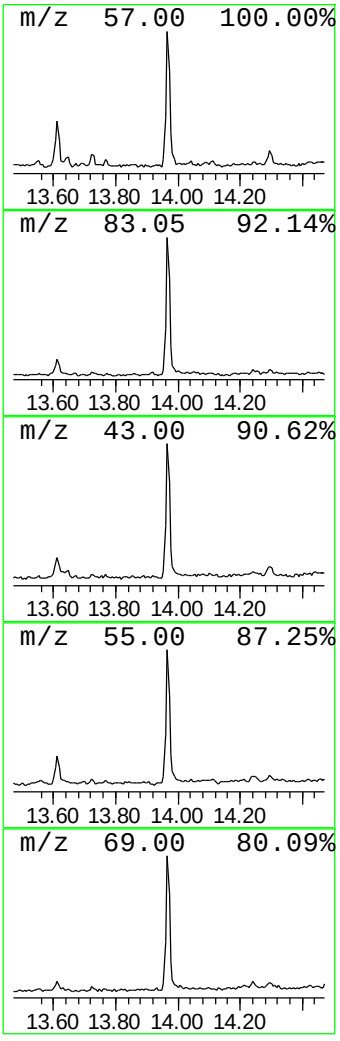
Peak Number 6 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	6.84 ng	532001	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	91
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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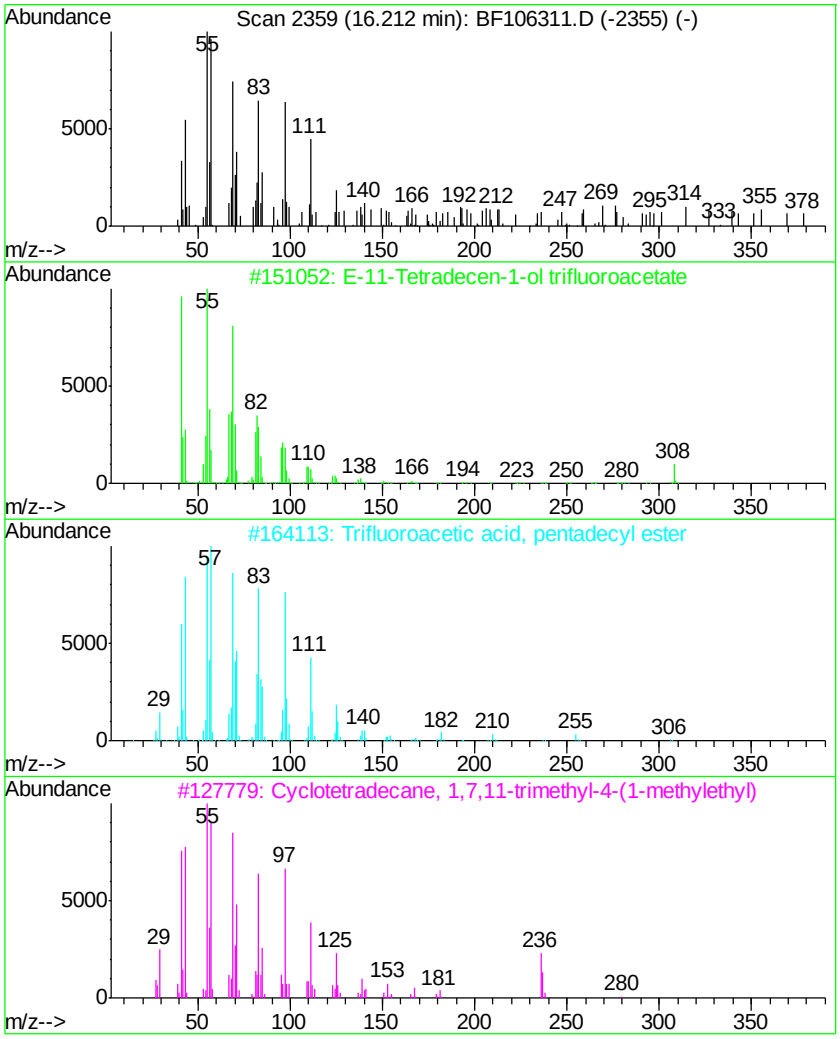
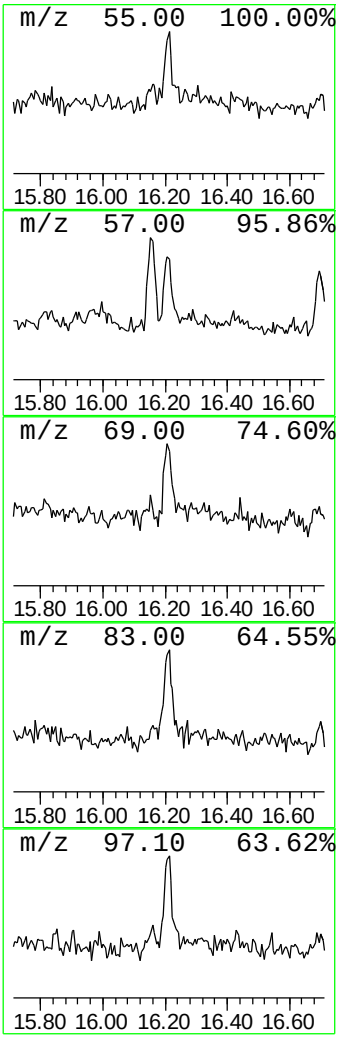
Peak Number 7 E-11-Tetradecen-1-ol triflu... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.21	2.02 ng	113366	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-11-Tetradecen-1-ol trifluoroac...	308	C16H27F3O2	1000130-84-1	86
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	80
3	Cyclotetradecane, 1,7,11-trimeth...	280	C20H40	001786-12-5	68
4	1-Docosene	308	C22H44	001599-67-3	50
5	1-Cyclohexyl-1-(4-methylcyclohex...	208	C15H28	002027-12-5	49





Tentatively Identified Compound (LSC) summary

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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
2-Pentanone, 4-hy...	5.20	5.8	ng	350082	1	6.97	1209090	20.0
unknown6.74	6.74	60.6	ng	3663520	1	6.97	1209090	20.0
n-Hexadecanoic acid	12.01	13.6	ng	836600	4	11.50	1228880	20.0
Octadecanoic acid	12.80	7.0	ng	428771	4	11.50	1228880	20.0
Behenic alcohol	13.97	6.8	ng	532001	5	14.15	1555340	20.0
E-11-Tetradecen-1...	16.21	2.0	ng	113366	6	15.68	1123520	20.0