LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081718\
Data File : BF108245.D
Acq On : 17 Aug 2018 16:09
Operator : JU/SJ
Sample : J4500-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

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-BF080818.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	5.248	490	495	506	rBV	588513	633992	21.61%	2.290%
2	5.636	557	561	565	rBV	2478818	2300887	78.42%	8.311%
3	6.631	725	730	743	rBV	2825206	2679712	91.33%	9.679%
4	6.783	752	756	759	rBV	2984756	2568221	87.53%	9.277%
5	7.013	792	795	799	rBV	1063301	857070	29.21%	3.096%
6	7.172	818	822	825	rBV	2501118	2020432	68.86%	7.298%
7	7.578	886	891	894	rBV	1715498	1670764	56.94%	6.035%
8	8.301	1010	1014	1017	rBV	1163971	1081505	36.86%	3.907%
9	9.372	1192	1196	1199	rBV	3572571	2934127	100.00%	10.598%
10	9.760	1259	1262	1268	rVB	213070	167135	5.70%	0.604%
11	10.060	1309	1313	1324	rVB	1450071	1238594	42.21%	4.474%
12	10.854	1444	1448	1461	rBV	1531844	1562362	53.25%	5.643%
13	10.954	1461	1465	1473	rVB	81516	90450	3.08%	0.327%
14	11.554	1563	1567	1570	rBV	1390991	1232111	41.99%	4.451%
15	11.577	1570	1571	1575	rVB	73054	48292	1.65%	0.174%
16	12.771	1771	1774	1778	rBV	79312	75950	2.59%	0.274%
17	13.007	1808	1814	1819	rBV	89801	107493	3.66%	0.388%
18	13.142	1833	1837	1840	rBV	3391261	2822777	96.21%	10.196%
19	14.059	1989	1993	2001	rBV3	67130	132000	4.50%	0.477%
20	14.212	2014	2019	2022	rBV	1205658	1223410	41.70%	4.419%
21	14.342	2038	2041	2045	rBV	50918	53194	1.81%	0.192%
22	14.648	2091	2093	2100	rVB2	46294	53327	1.82%	0.193%
23	14.977	2146	2149	2153	rVB	68107	64733	2.21%	0.234%
24	15.065	2160	2164	2169	rVB	126720	143970	4.91%	0.520%
25	15.301	2201	2204	2207	rBV	37134	49208	1.68%	0.178%
26	15.342	2209	2211	2215	rVB	77148	83625	2.85%	0.302%
27	15.701	2269	2272	2277	rBV	36749	55908	1.91%	0.202%
28	15.771	2278	2284	2294	rVB2	829771	1222937	41.68%	4.417%
29	16.242	2359	2364	2370	rVB	91720	144102	4.91%	0.521%
30	16.795	2454	2458	2466	rVB2	76324	134709	4.59%	0.487%
31	17.453	2566	2570	2577	rVB2	53337	113469	3.87%	0.410%
32	18.236	2699	2703	2712	rVB3	48126	118165	4.03%	0.427%

LSC Area Percent Report

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Misc :
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Instrument :
BNA_F
ClientSampleId :
TP-1

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-BF080818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 27684631

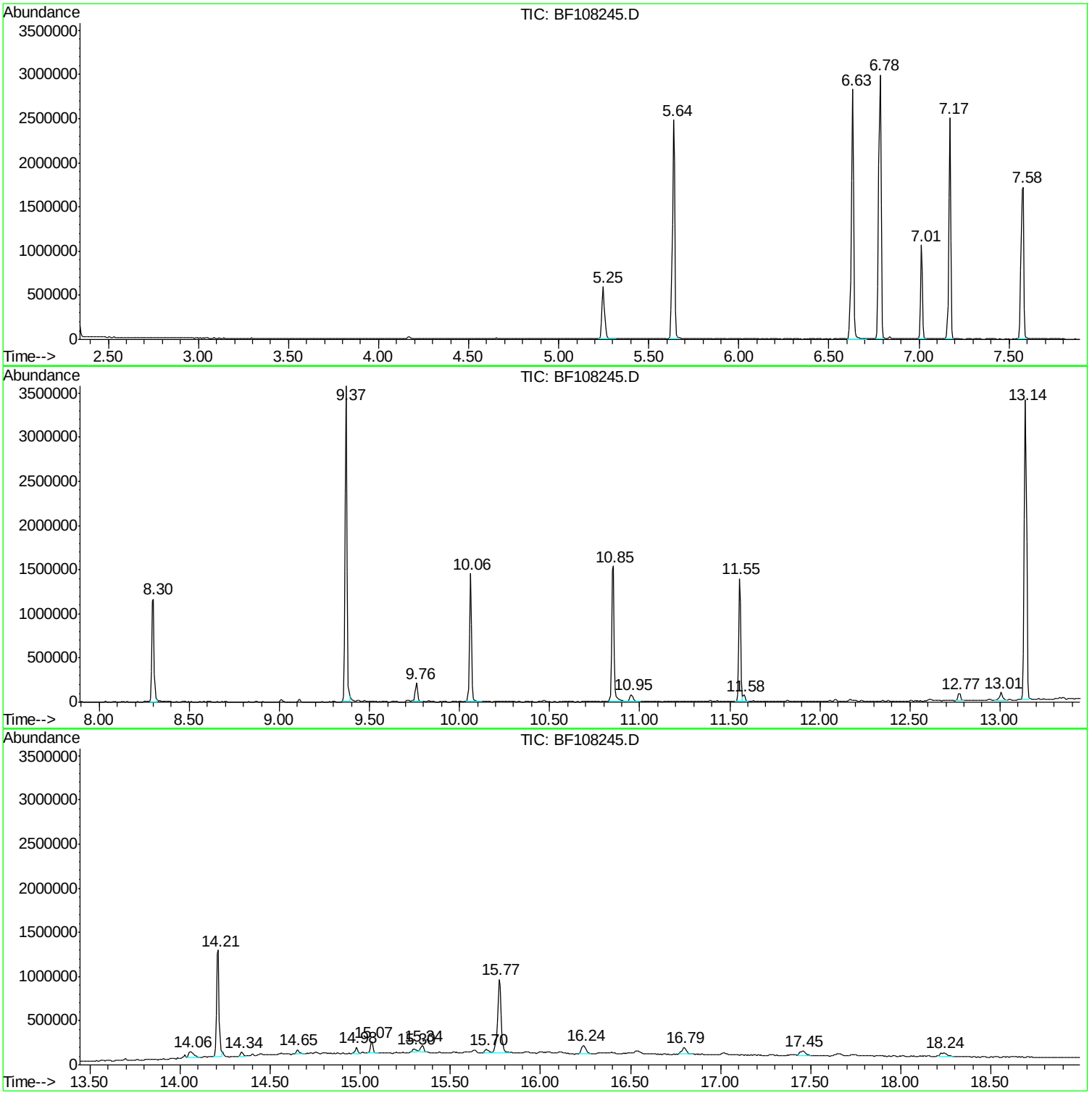
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081718\
Data File : BF108245.D
Acq On : 17 Aug 2018 16:09
Operator : JU/SJ
Sample : J4500-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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\BF081718\
Data File : BF108245.D
Acq On : 17 Aug 2018 16:09
Operator : JU/SJ
Sample : J4500-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

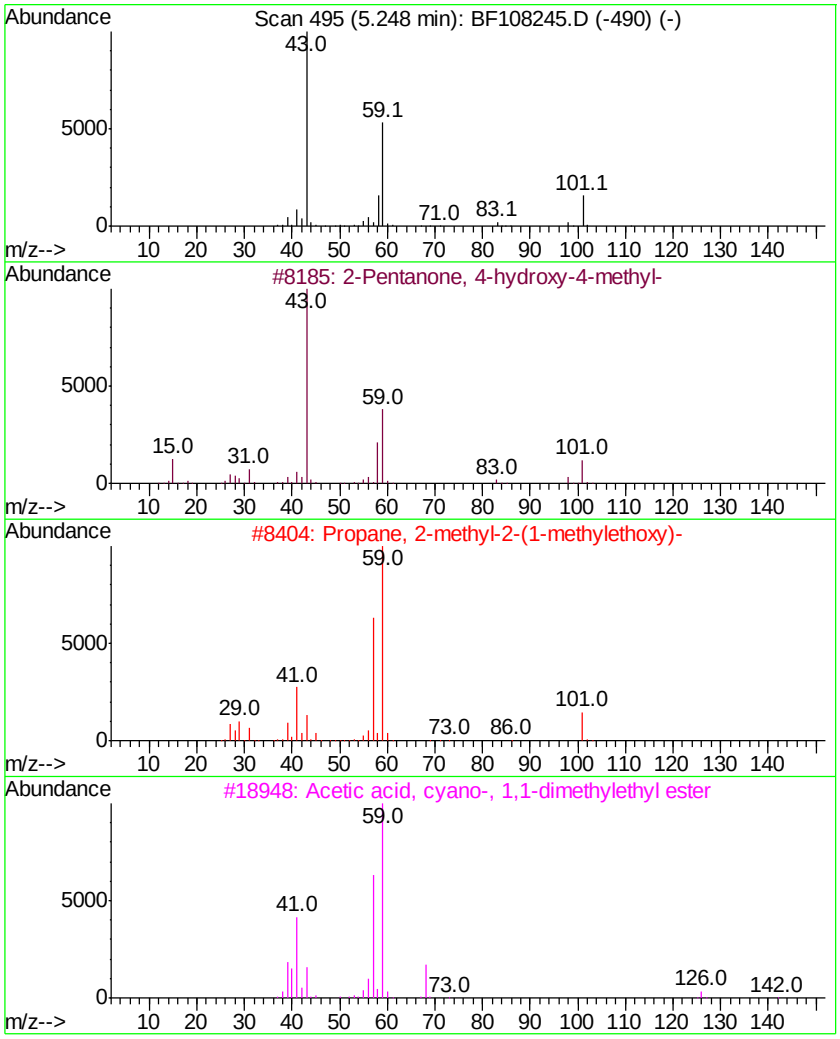
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

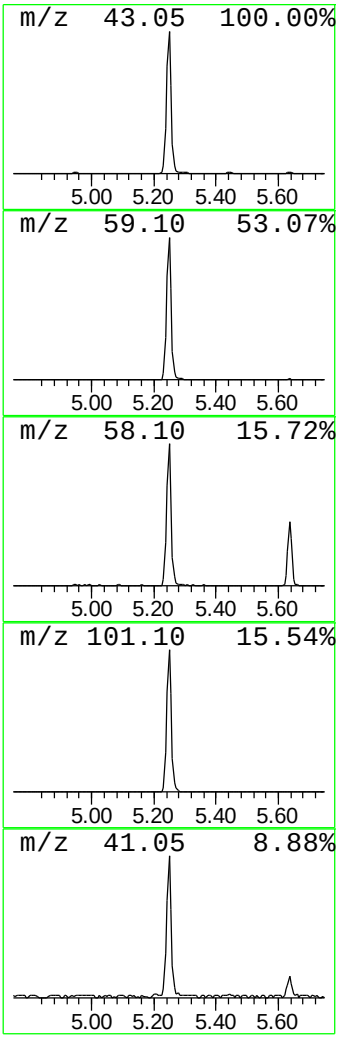
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.25	14.79 ng	633992	1,4-Dichlorobenzene-d4	7.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081718\
Data File : BF108245.D
Acq On : 17 Aug 2018 16:09
Operator : JU/SJ
Sample : J4500-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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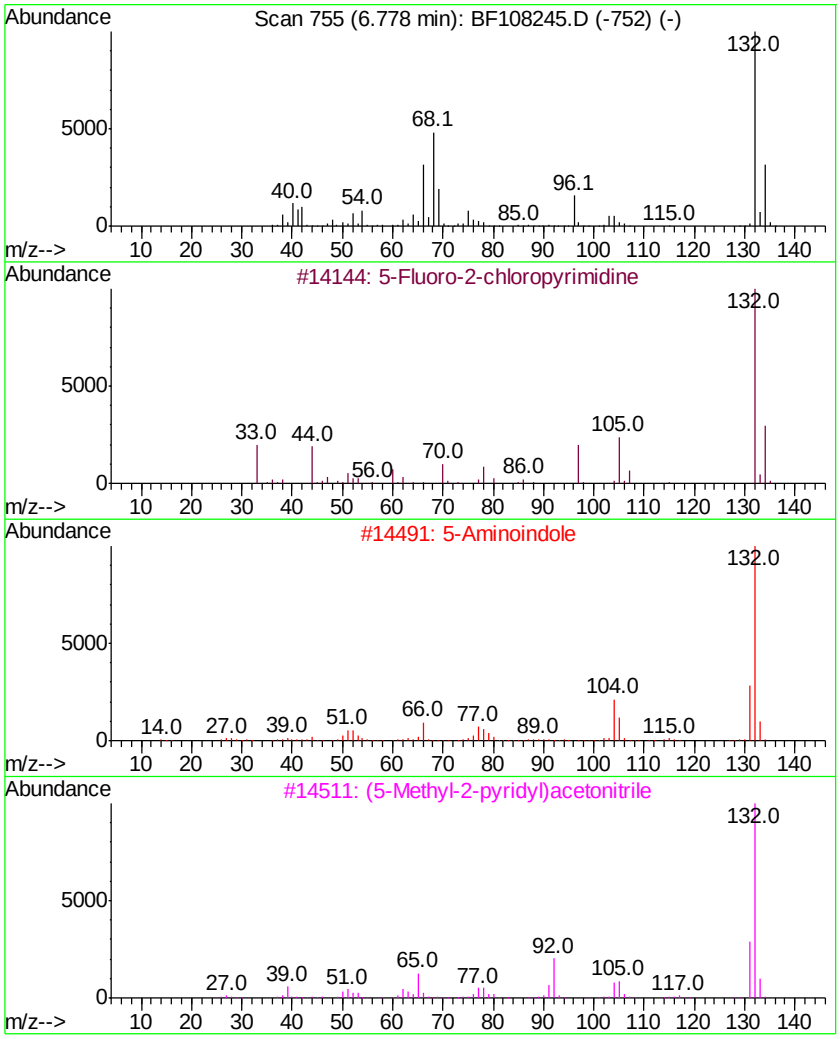
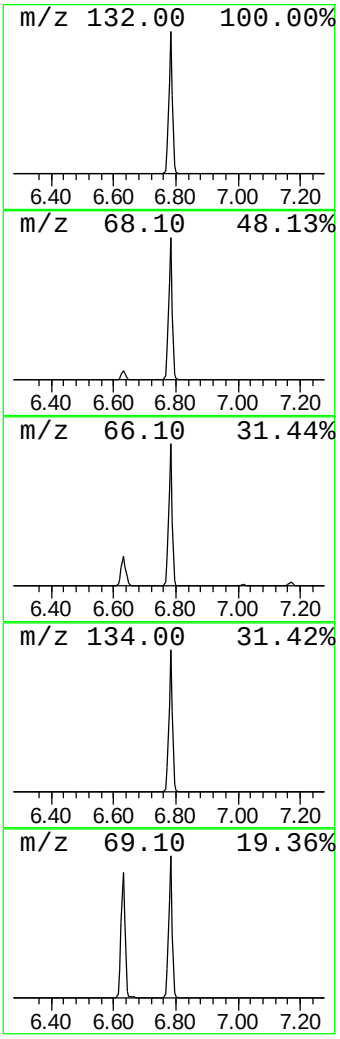
Peak Number 2 unknown6.78 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	59.93 ng	2568220	1,4-Dichlorobenzene-d4	7.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Operator : JU/SJ
Sample : J4500-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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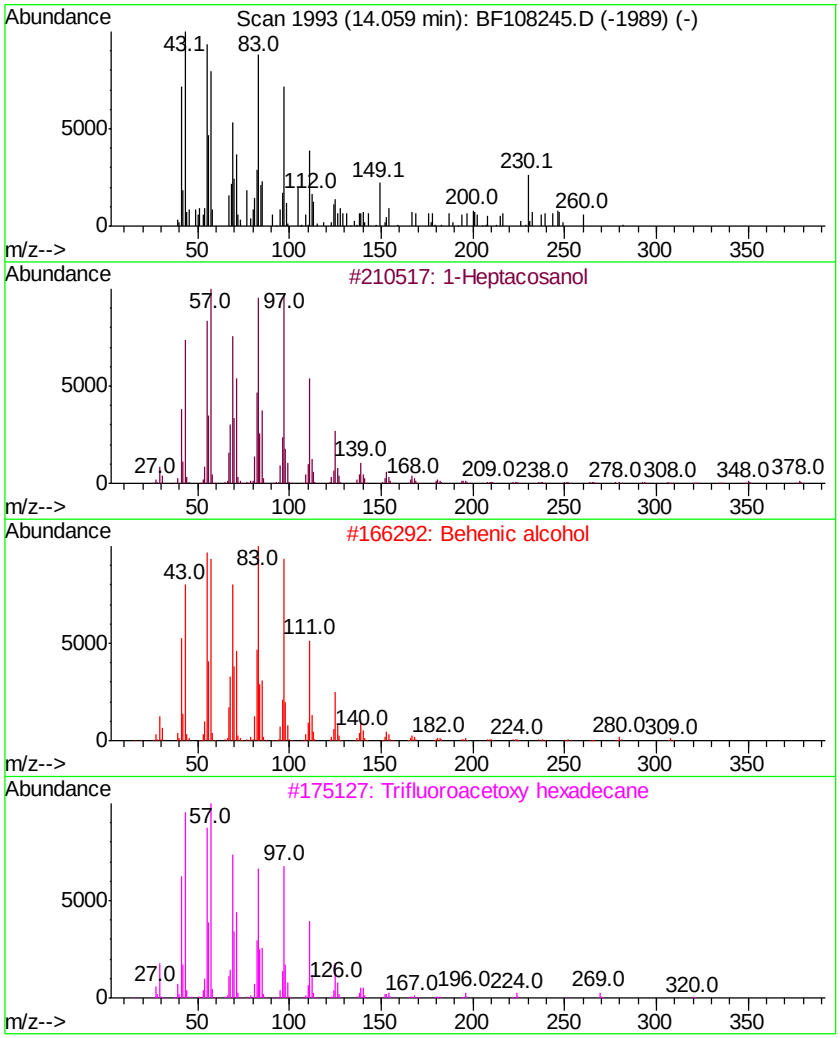
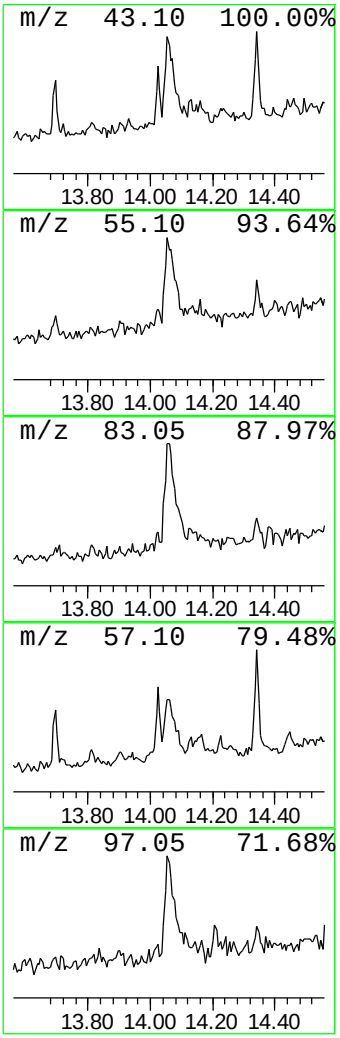
Peak Number 4 1-Heptacosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.06	2.16 ng	132000	Chrysene-d12	14.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	68
2	Behenic alcohol	326	C22H46O	000661-19-8	60
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	60
4	1-Heneicosanol	312	C21H44O	015594-90-8	60
5	1-Docosene	308	C22H44	001599-67-3	60





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081718\
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Misc :
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Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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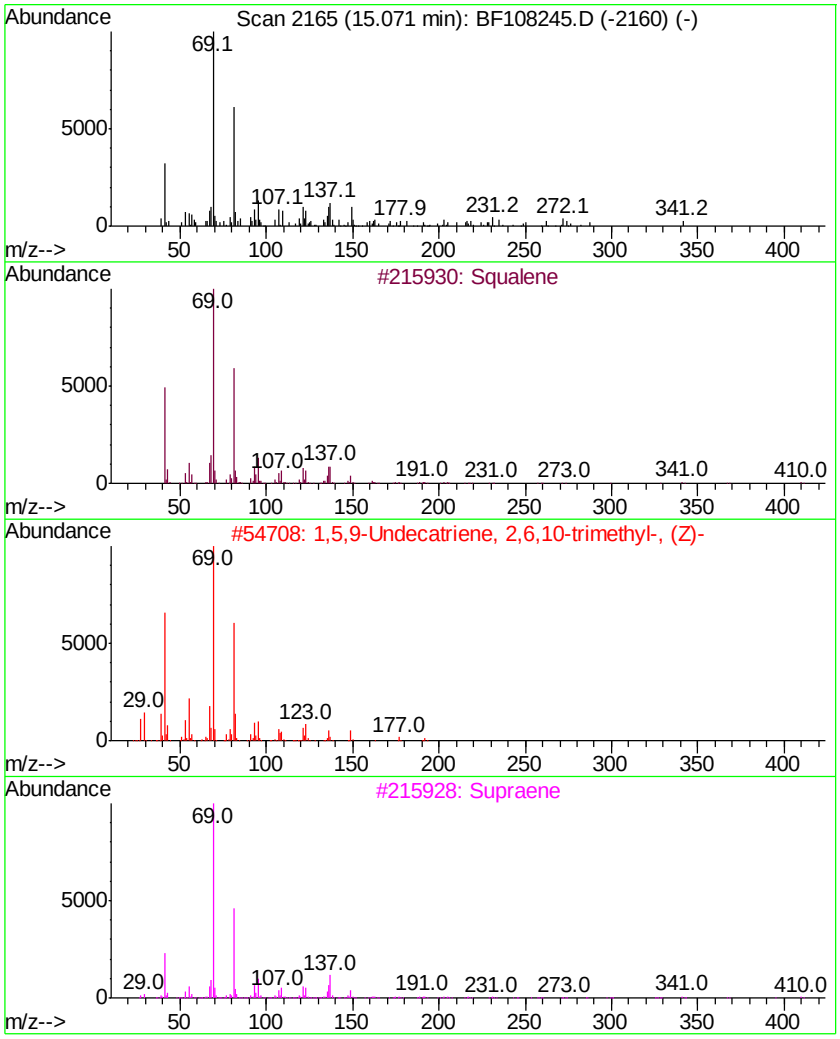
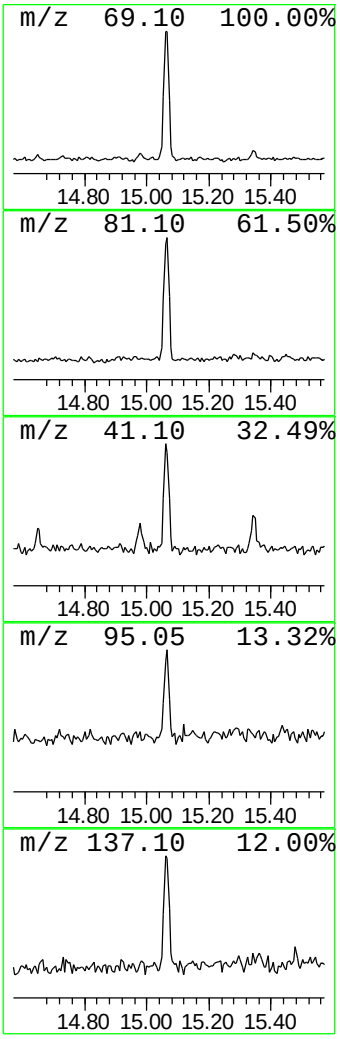
Peak Number 5 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	2.35 ng	143970	Perylene-d12	15.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	87
2	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	74
3	Supraene	410	C30H50	007683-64-9	72
4	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	64
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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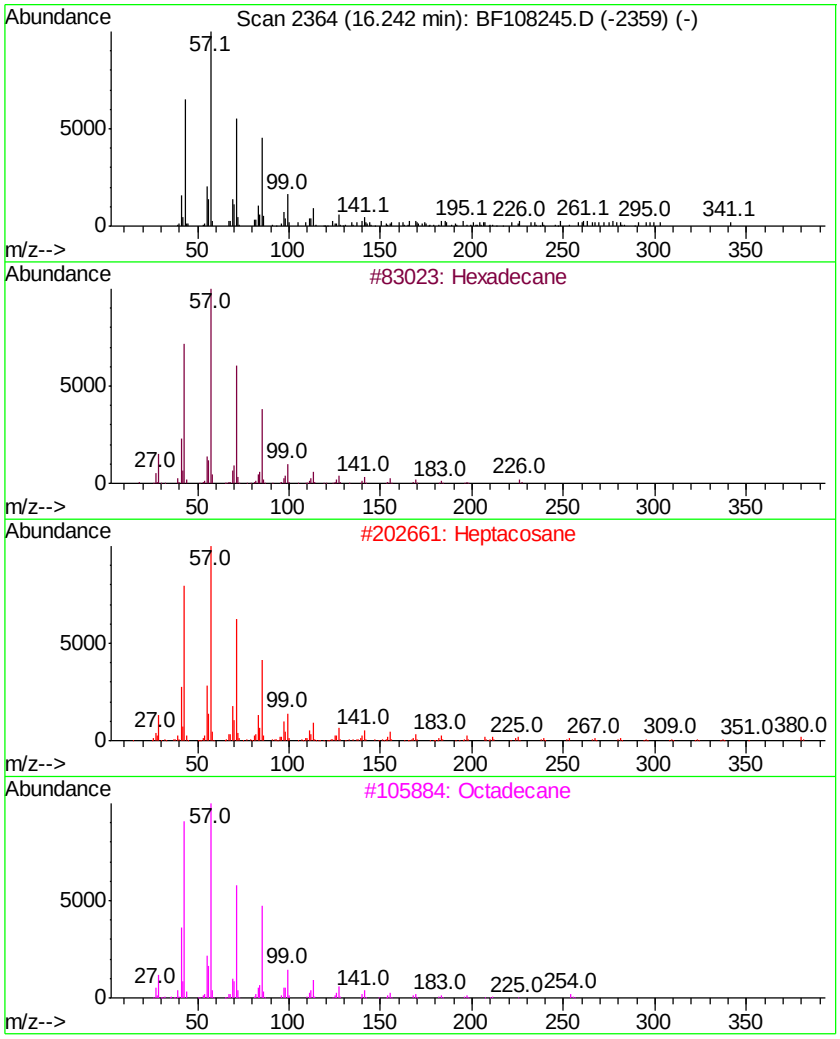
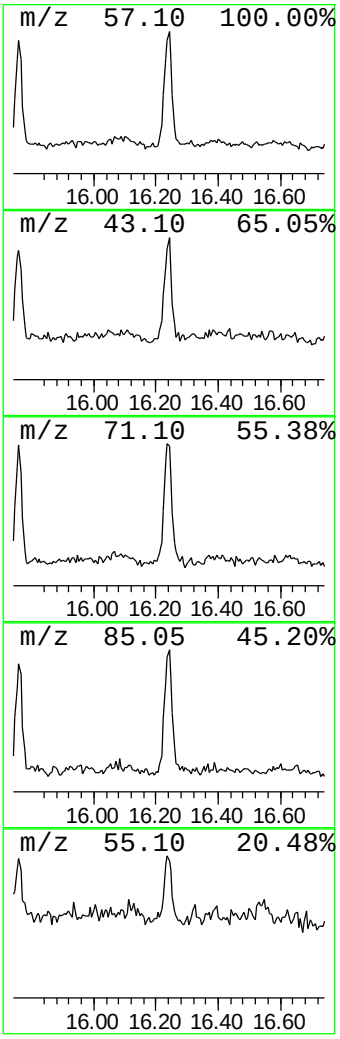
Peak Number 6 Hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.24	2.36 ng	144102	Perylene-d12	15.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	93
2	Heptacosane	380	C27H56	000593-49-7	90
3	Octadecane	254	C18H38	000593-45-3	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Heneicosane	296	C21H44	000629-94-7	90





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Instrument : BNA_F
ClientSampleId : TP-1

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TIC Library : C:\DATABASE\NIST11.L
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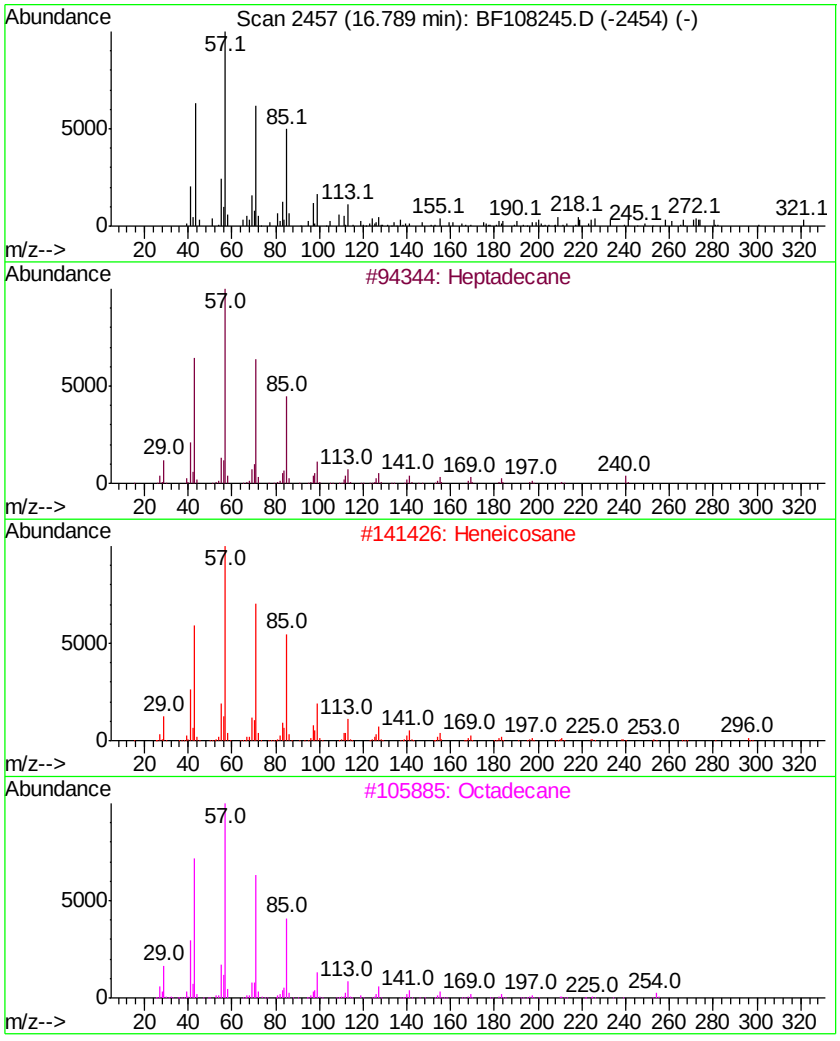
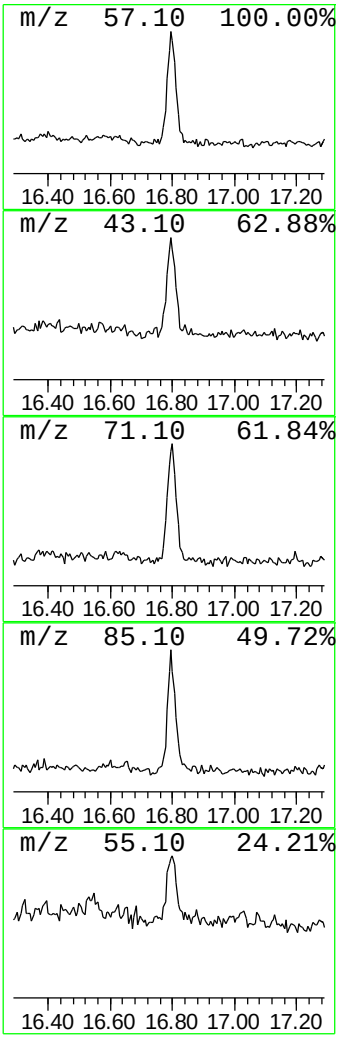
Peak Number 7 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.79	2.20 ng	134709	Perylene-d12	15.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	94
2	Heneicosane	296	C21H44	000629-94-7	94
3	Octadecane	254	C18H38	000593-45-3	93
4	Octacosane	394	C28H58	000630-02-4	83
5	6,6-Diethylhoctadecane	310	C22H46	1000360-41-8	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081718\
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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...	5.25	14.8	ng	633992	1	7.01	857070	20.0
unknown6.78	6.78	59.9	ng	2568220	1	7.01	857070	20.0
1-Heptacosanol	14.06	2.2	ng	132000	5	14.21	1223410	20.0
Squalene	15.07	2.4	ng	143970	6	15.77	1222940	20.0
Hexadecane	16.24	2.4	ng	144102	6	15.77	1222940	20.0
Heptadecane	16.79	2.2	ng	134709	6	15.77	1222940	20.0