LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF083117\
Data File : BF098211.D
Acq On : 31 Aug 2017 22:59
Operator : SJ/JU
Sample : I4963-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3830-PA2

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-BF081517.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	4.910	476	480	490	rVB	82923	108375	2.82%	0.407%
2	5.328	547	551	555	rBV	1566150	1558379	40.57%	5.847%
3	6.363	720	727	736	rBV	1082524	1122930	29.23%	4.214%
4	6.492	744	749	752	rBV	2810934	2655232	69.12%	9.963%
5	6.716	783	787	791	rBV	956182	781055	20.33%	2.931%
6	6.875	809	814	817	rBV	2715522	2487510	64.75%	9.334%
7	6.910	817	820	832	rVB	63974	72083	1.88%	0.270%
8	7.286	878	884	887	rBV	2162919	2217588	57.73%	8.321%
9	7.792	966	970	975	rBV	38674	40896	1.06%	0.153%
10	8.004	1001	1006	1009	rBV	1071717	1061258	27.63%	3.982%
11	8.280	1049	1053	1057	rBV	230457	211609	5.51%	0.794%
12	9.080	1183	1189	1192	rBV	3695006	3841587	100.00%	14.415%
13	9.751	1298	1303	1307	rBV	1308121	1226608	31.93%	4.603%
14	10.545	1432	1438	1441	rBV	2125235	2196502	57.18%	8.242%
15	10.657	1453	1457	1461	rBV	68816	76758	2.00%	0.288%
16	11.233	1551	1555	1559	rBV	1363967	1267366	32.99%	4.756%
17	11.957	1675	1678	1685	rVB	41628	50090	1.30%	0.188%
18	12.827	1820	1826	1829	rBV	3391388	3609401	93.96%	13.543%
19	13.868	1999	2003	2009	rVB	929865	835796	21.76%	3.136%
20	15.286	2239	2244	2247	rBV	515792	635780	16.55%	2.386%
21	15.721	2314	2318	2324	rVB	88908	133799	3.48%	0.502%
22	16.186	2393	2397	2403	rVB	100797	171262	4.46%	0.643%
23	16.733	2485	2490	2498	rVB3	74070	149624	3.89%	0.561%
24	17.380	2596	2600	2607	rVB3	67582	139027	3.62%	0.522%

Sum of corrected areas: 26650515

LSC Report - Integrated Chromatogram

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Misc :
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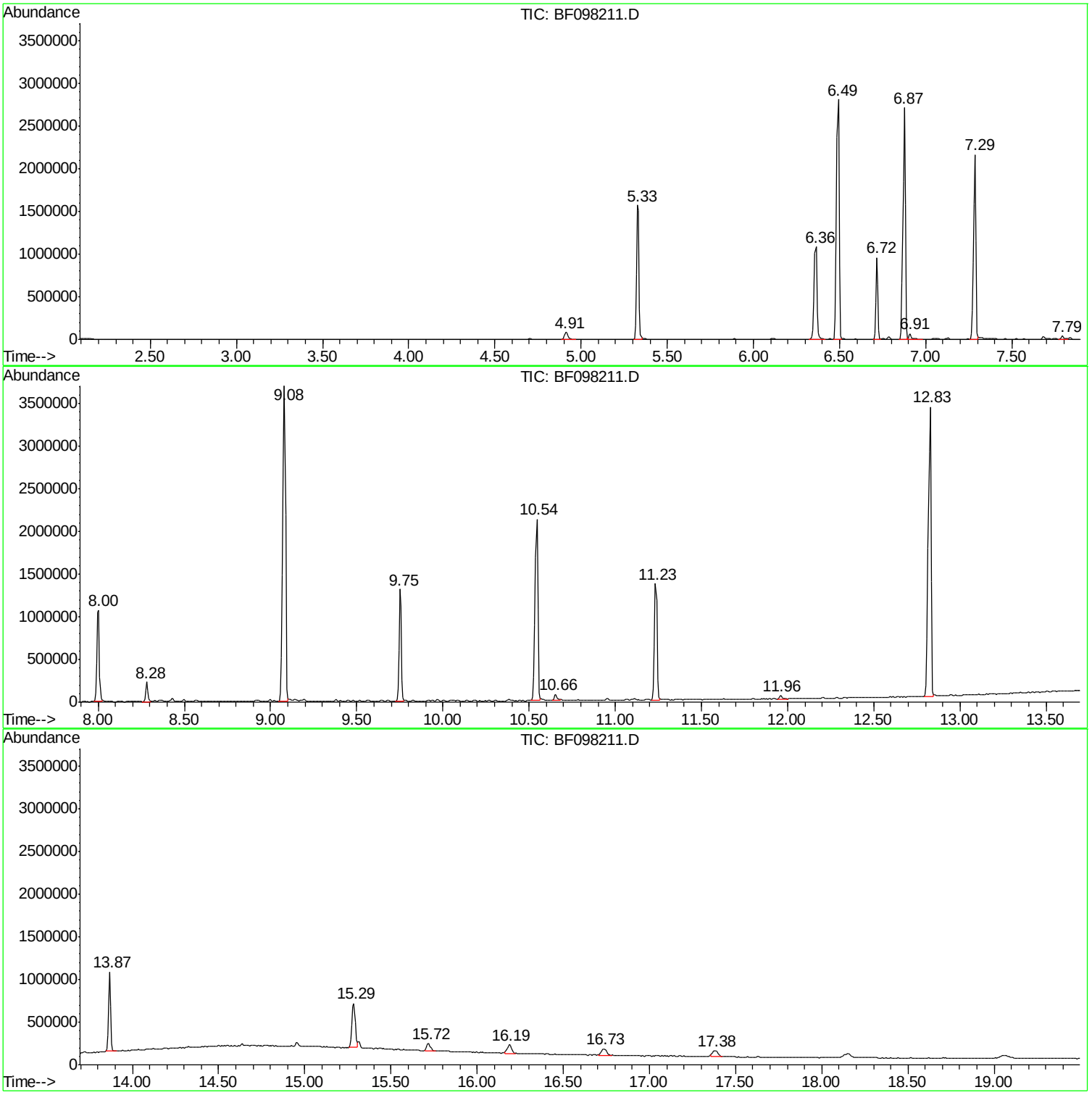
Instrument : BNA_F
ClientSampleId : 3830-PA2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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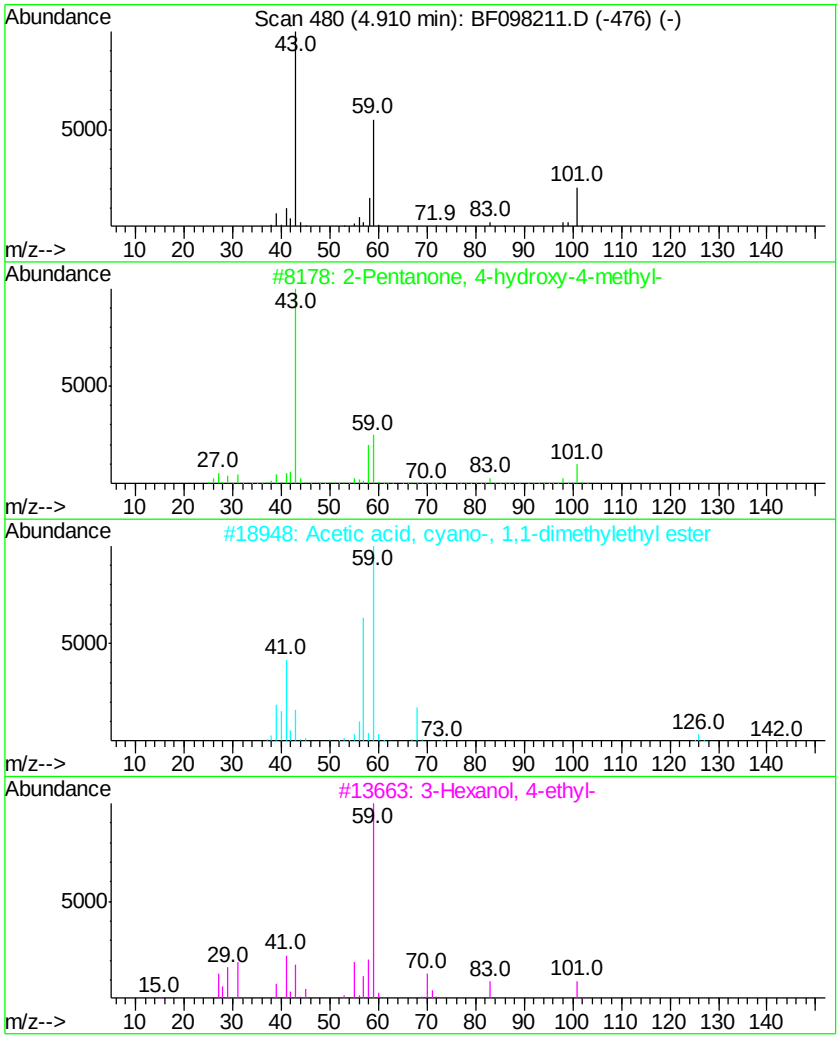
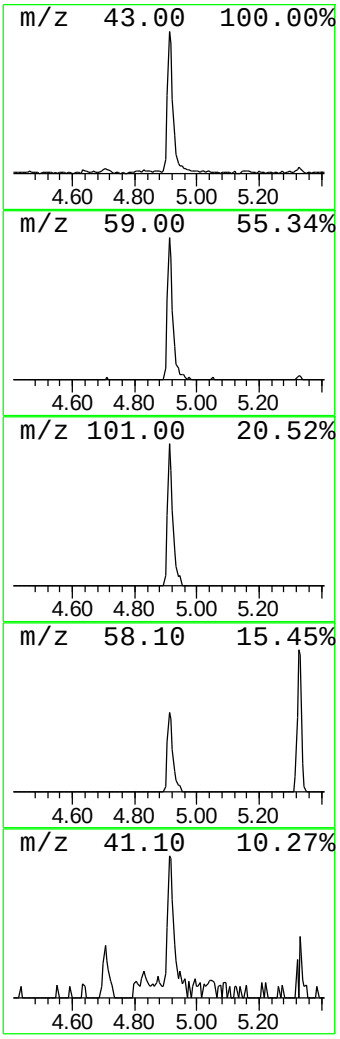
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	2.78 ng	108375	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3	3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	28
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25





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Instrument : BNA_F
ClientSampleId : 3830-PA2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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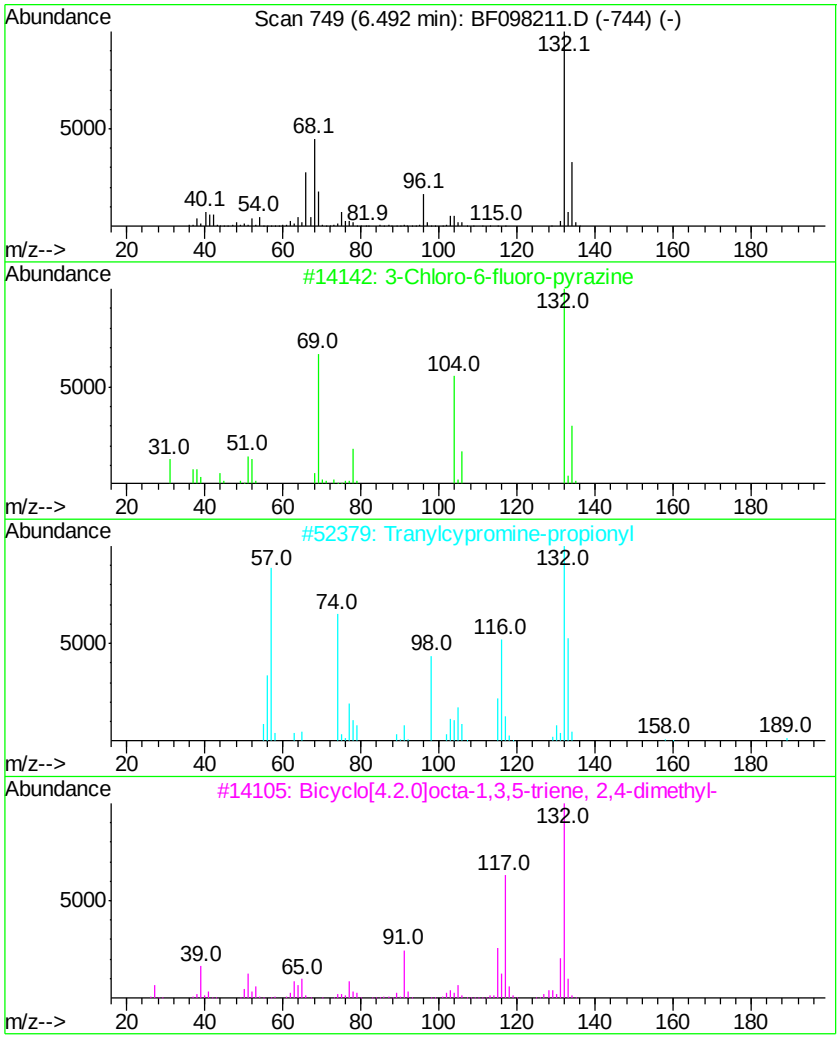
Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	67.99 ng	2655230	1,4-Dichlorobenzene-d4	6.72

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	Xenon	132	Xe	007440-63-3	9
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9



m/z 132.10 100.00%

m/z 68.10 44.91%

m/z 134.00 32.84%

m/z 66.00 27.78%

m/z 69.10 17.89%

Data Path : Z:\HPCHEM1\BNA F\DATA\BF083117\
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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3830-PA2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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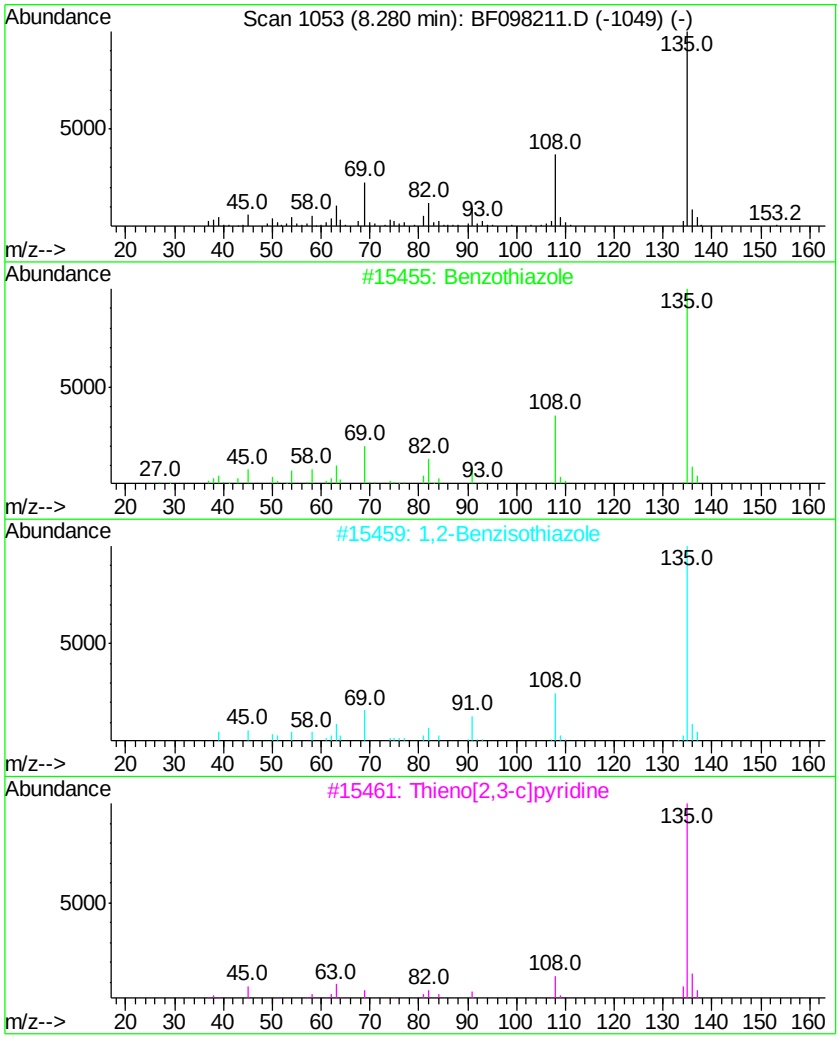
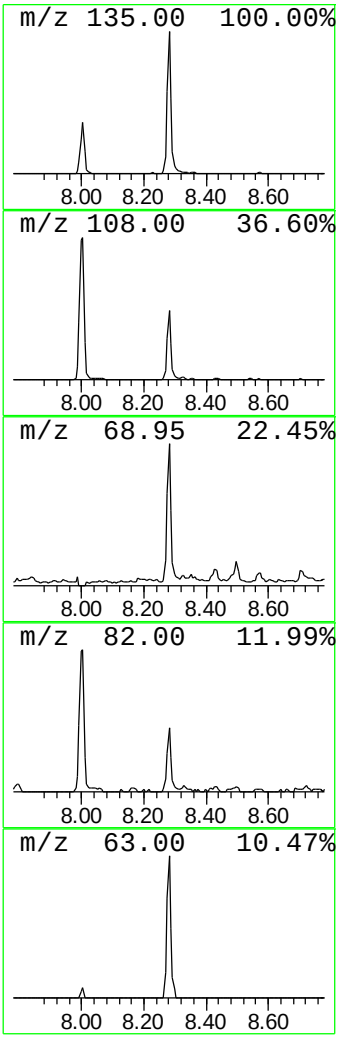
Peak Number 4 Benzothiazole Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.28	3.99 ng	211609	Naphthalene-d8	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole	135	C7H5NS	000095-16-9	97
2	1,2-Benzisothiazole	135	C7H5NS	000272-16-2	87
3	Thieno[2,3-c]pyridine	135	C7H5NS	000272-12-8	72
4	3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	56
5	Adenine	135	C5H5N5	000073-24-5	53





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Operator : SJ/JU
Sample : I4963-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3830-PA2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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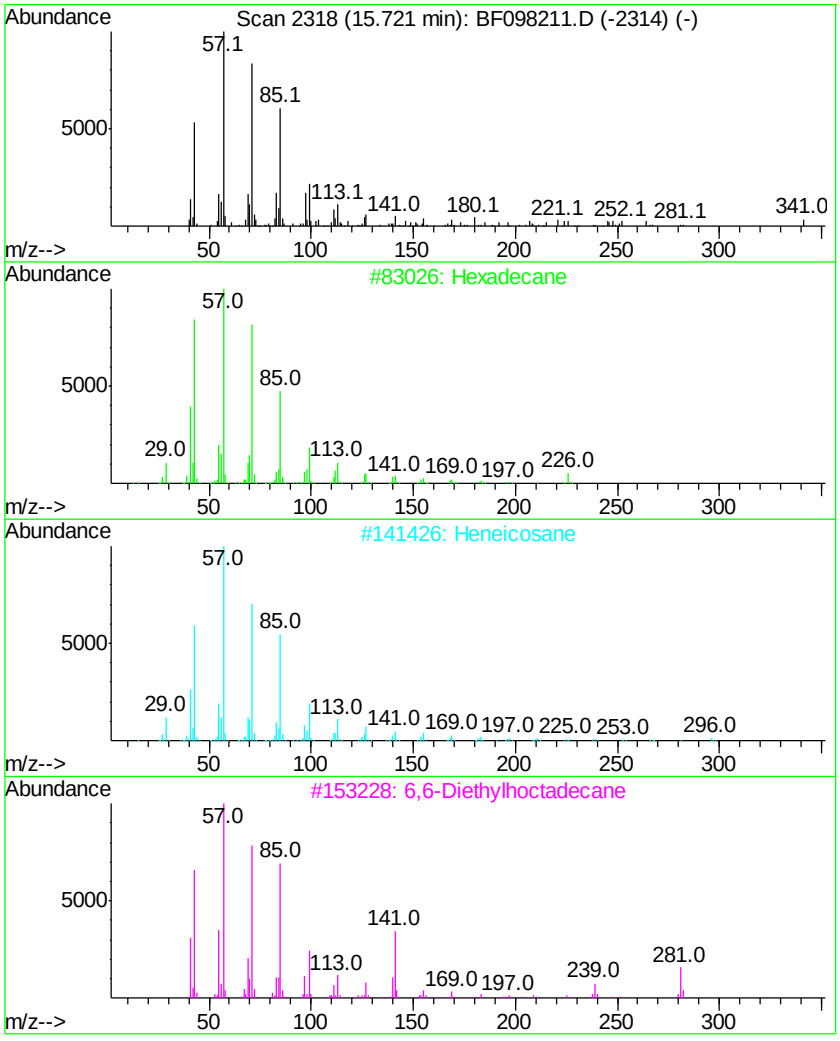
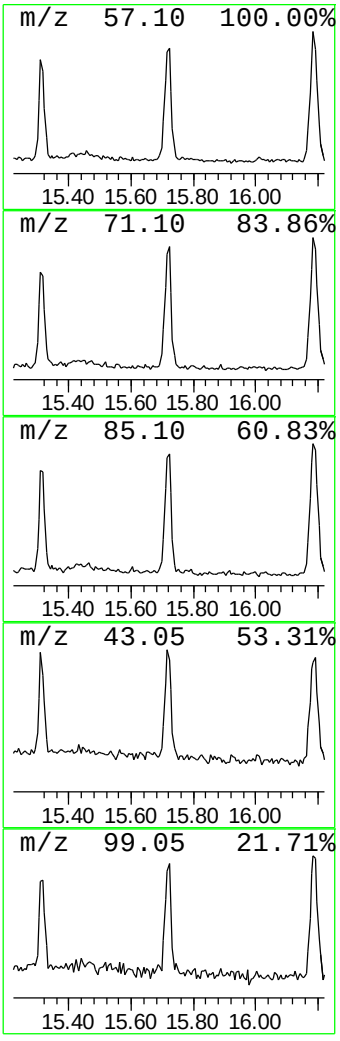
Peak Number 5 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	4.21 ng	133799	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	6,6-Diethylhoctadecane	310	C22H46	1000360-41-8	90
4	Tetracosane	338	C24H50	000646-31-1	87
5	Hexacosane	366	C26H54	000630-01-3	86





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF083117\
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Acq On : 31 Aug 2017 22:59
Operator : SJ/JU
Sample : I4963-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3830-PA2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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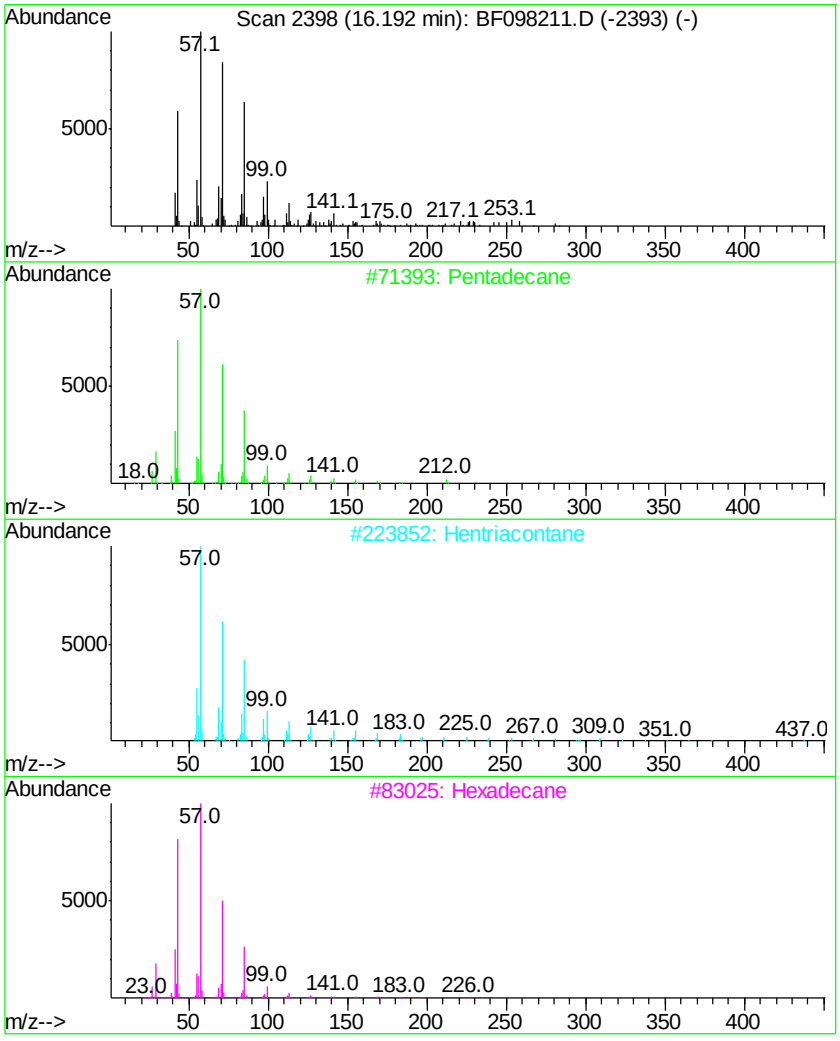
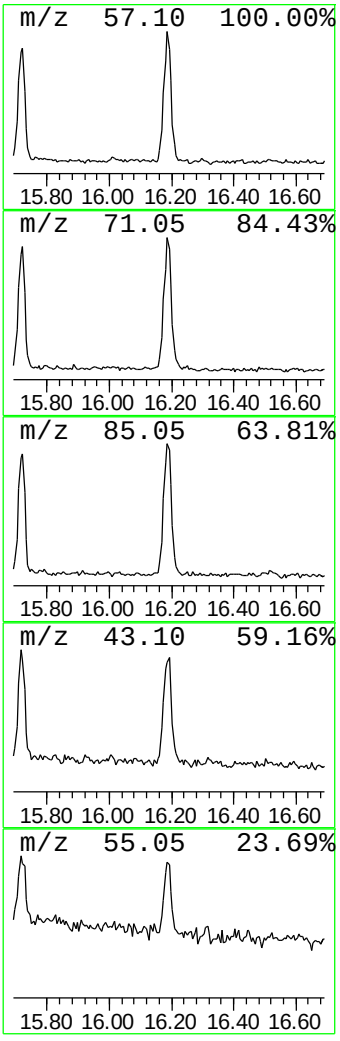
Peak Number 6 Pentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	5.39 ng	171262	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	90
2	Hentriacontane	437	C31H64	000630-04-6	90
3	Hexadecane	226	C16H34	000544-76-3	89
4	Hexacosane	366	C26H54	000630-01-3	87
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86





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Instrument : BNA_F
ClientSampleId : 3830-PA2

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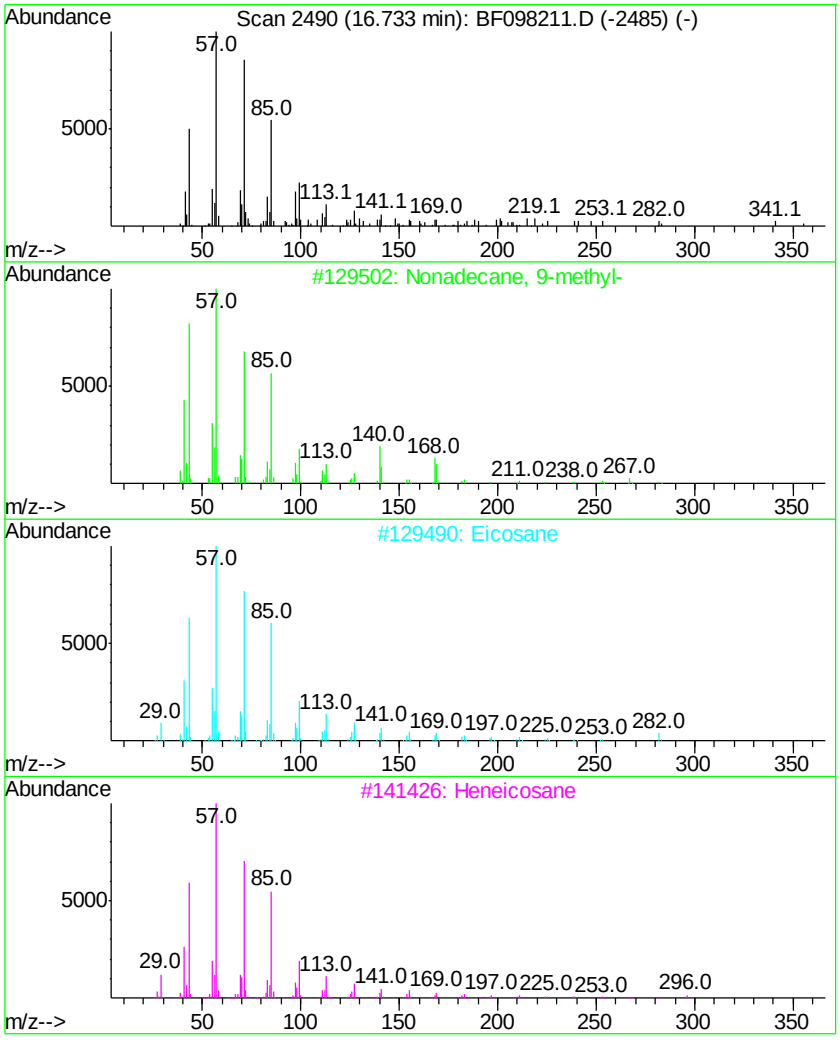
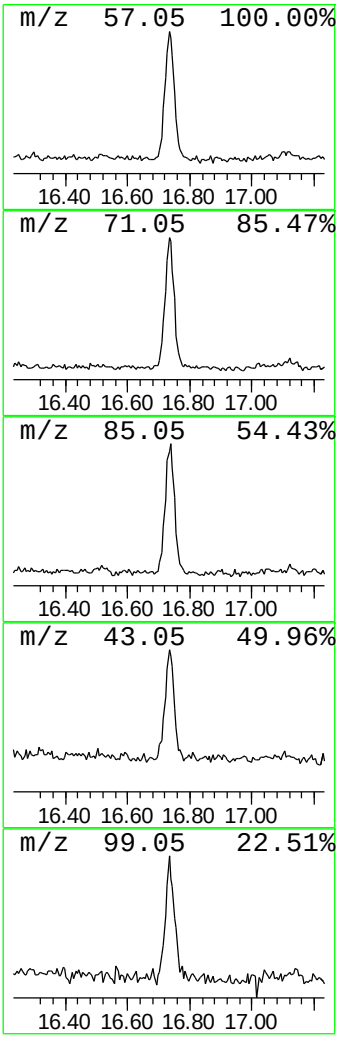
Peak Number 7 Nonadecane, 9-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.73	4.71 ng	149624	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	91
2	Eicosane	282	C20H42	000112-95-8	90
3	Heneicosane	296	C21H44	000629-94-7	87
4	Dodecane, 2-methyl-	184	C13H28	001560-97-0	87
5	Triacontane	422	C30H62	000638-68-6	86





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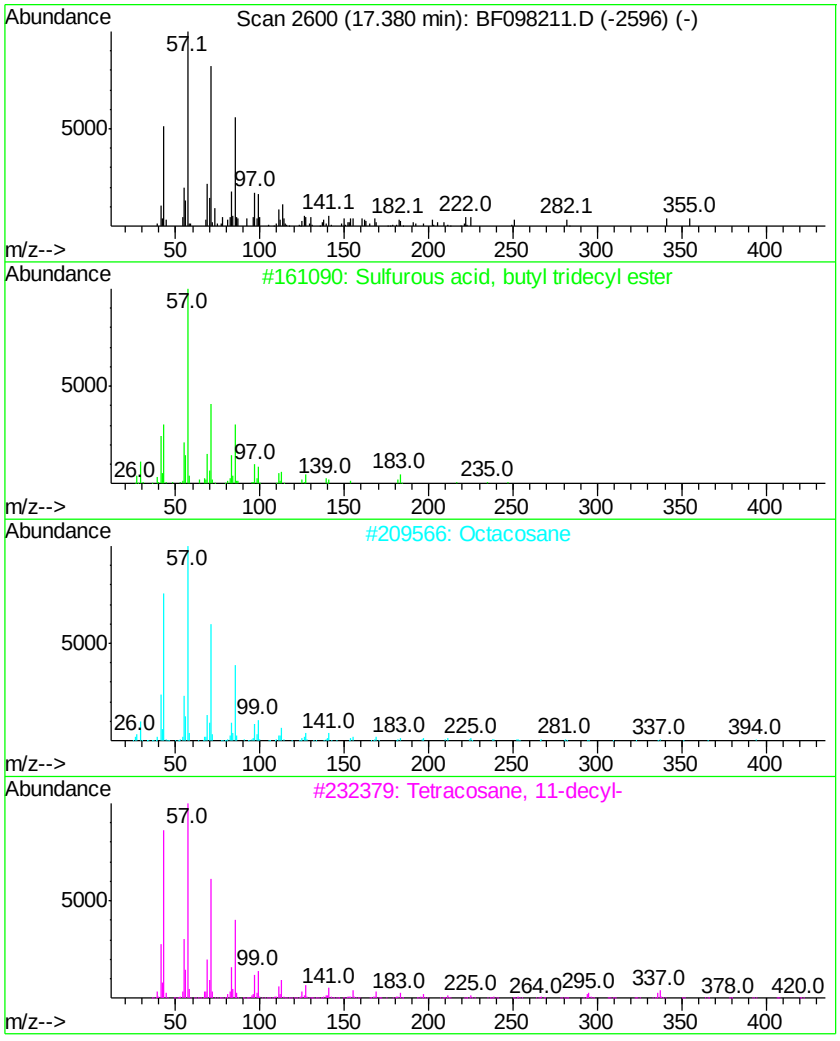
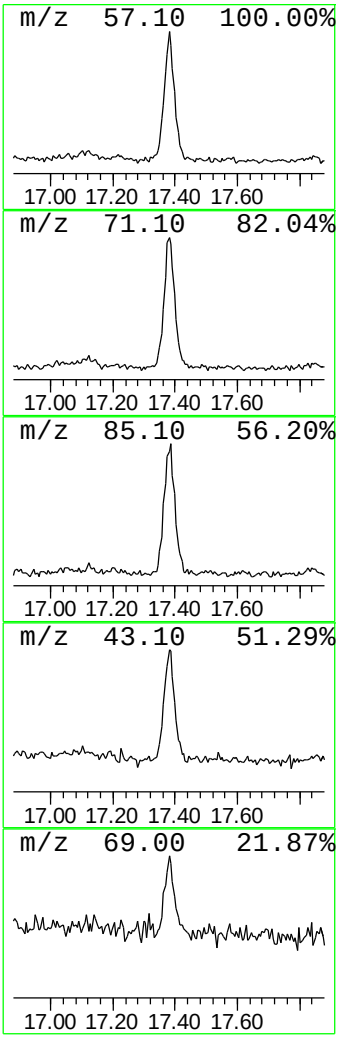
Peak Number 8 Sulfurous acid, butyl tride... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.38	4.37 ng	139027	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	80
2	Octacosane	394	C28H58	000630-02-4	80
3	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	80
4	Heptacosane	380	C27H56	000593-49-7	80
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	80





Tentatively Identified Compound (LSC) summary

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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...	4.91	2.8	ng	108375	1	6.72	781055	20.0
unknown6.49	6.49	68.0	ng	2655230	1	6.72	781055	20.0
Benzothiazole	8.28	4.0	ng	211609	2	8.00	1061260	20.0
Hexadecane	15.72	4.2	ng	133799	6	15.29	635780	20.0
Pentadecane	16.19	5.4	ng	171262	6	15.29	635780	20.0
Nonadecane, 9-met...	16.73	4.7	ng	149624	6	15.29	635780	20.0
Sulfurous acid, b...	17.38	4.4	ng	139027	6	15.29	635780	20.0