LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108535.D
Acq On : 28 Aug 2018 3:15
Operator : JU/SJ
Sample : J4659-08
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082218-SIDI-E-U-S

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	5.231	489	492	499	rVB	34678	39432	1.11%	0.196%
2	5.625	555	559	573	rBV	967009	918447	25.92%	4.563%
3	6.613	724	727	731	rBV	737516	645963	18.23%	3.209%
4	6.766	749	753	757	rBV	2044453	1737034	49.02%	8.630%
5	6.995	789	792	796	rBV	683192	620189	17.50%	3.081%
6	7.154	815	819	823	rBV	2654418	2492264	70.33%	12.383%
7	7.560	883	888	892	rBV	1949283	2012376	56.79%	9.998%
8	8.283	1007	1011	1026	rBV	817228	732355	20.67%	3.639%
9	9.354	1187	1193	1197	rBV	3756918	3543467	100.00%	17.605%
10	9.742	1256	1259	1265	rBV	63781	58696	1.66%	0.292%
11	10.042	1307	1310	1324	rVB2	813819	712898	20.12%	3.542%
12	10.442	1376	1378	1382	rVB	40966	36714	1.04%	0.182%
13	10.701	1418	1422	1426	rBV	99466	83609	2.36%	0.415%
14	10.836	1441	1445	1456	rBV	1137527	1123440	31.70%	5.582%
15	11.536	1560	1564	1572	rBV	729503	635771	17.94%	3.159%
16	13.124	1829	1834	1837	rBV	3130356	2758293	77.84%	13.704%
17	14.071	1989	1995	2001	rBV7	13726	40332	1.14%	0.200%
18	14.189	2011	2015	2025	rVB	771665	707014	19.95%	3.513%
19	14.624	2085	2089	2093	rVB	65177	64272	1.81%	0.319%
20	14.948	2140	2144	2148	rBV	103481	104726	2.96%	0.520%
21	15.312	2201	2206	2211	rVB	114694	139419	3.93%	0.693%
22	15.742	2270	2279	2294	rVB2	361400	652080	18.40%	3.240%
23	16.189	2350	2355	2362	rBV	86265	140127	3.95%	0.696%
24	16.742	2441	2449	2455	rBV2	47254	90127	2.54%	0.448%
25	17.389	2555	2559	2566	rVB4	17552	38189	1.08%	0.190%

Sum of corrected areas: 20127234

LSC Report - Integrated Chromatogram

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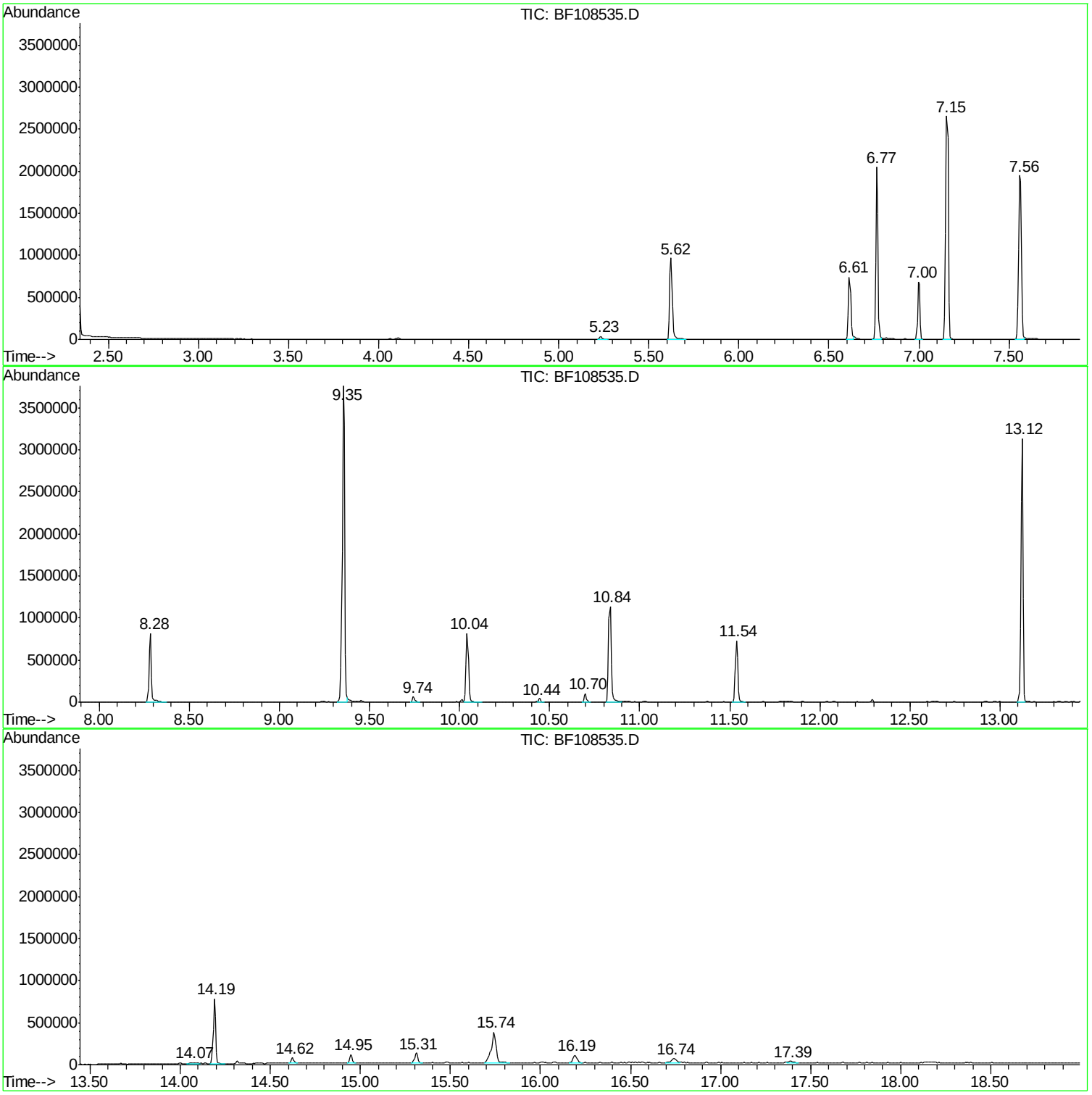
Instrument : BNA_F
ClientSampleId : 082218-SIDI-E-U-S

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

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Data File : BF108535.D
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Operator : JU/SJ
Sample : J4659-08
Misc :
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Instrument : BNA_F
ClientSampleId : 082218-SIDI-E-U-S

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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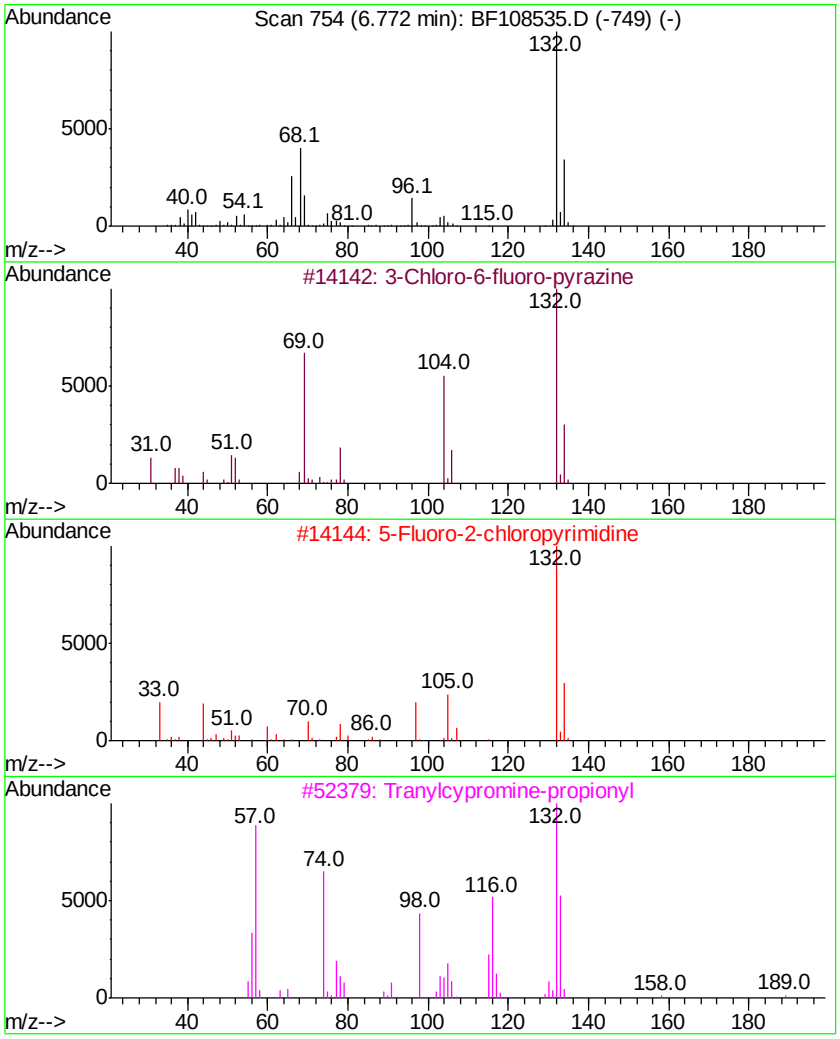
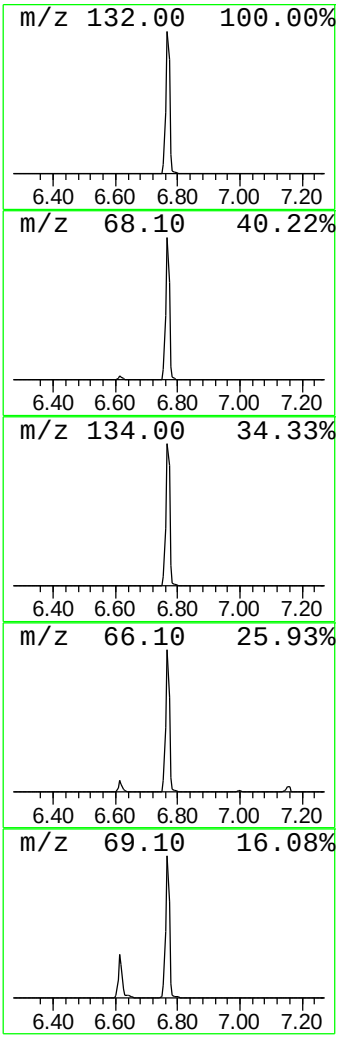
Peak Number 1 unknown6.77 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	56.02 ng	1737030	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Operator : JU/SJ
Sample : J4659-08
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082218-SIDI-E-U-S

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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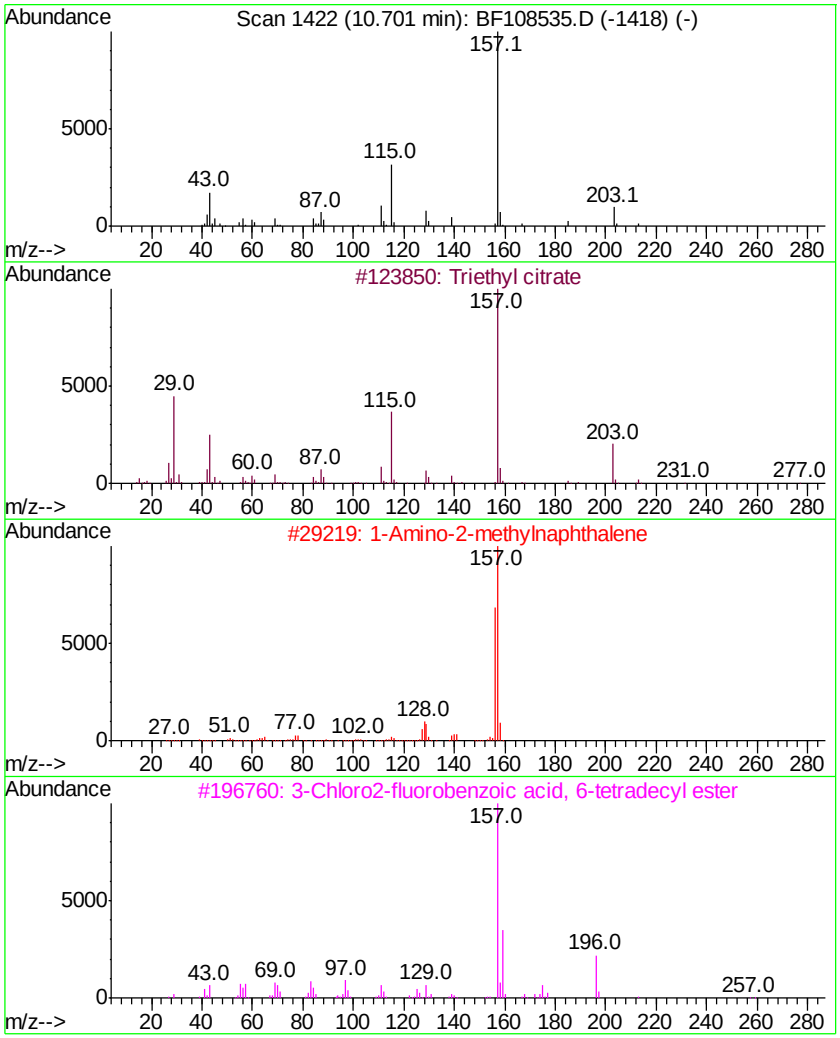
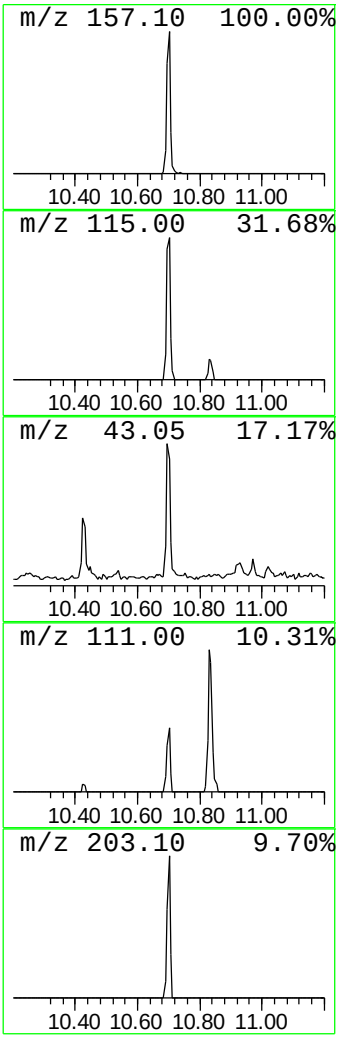
Peak Number 3 Triethyl citrate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	2.35 ng	83609	Acenaphthene-d10	10.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	86
2	1-Amino-2-methylnaphthalene	157	C11H11N	002246-44-8	38
3	3-Chloro2-fluorobenzoic acid, 6-...	370	C21H32ClFO2	1000338-64-9	36
4	3-Chloro2-fluorobenzoic acid, 4-...	370	C21H32ClFO2	1000338-64-7	36
5	Piperazine-1-carboxylic acid, 4-...	396	C14H18Cl2N2O5S	1000303-80-3	36





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108535.D
Acq On : 28 Aug 2018 3:15
Operator : JU/SJ
Sample : J4659-08
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082218-SIDI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
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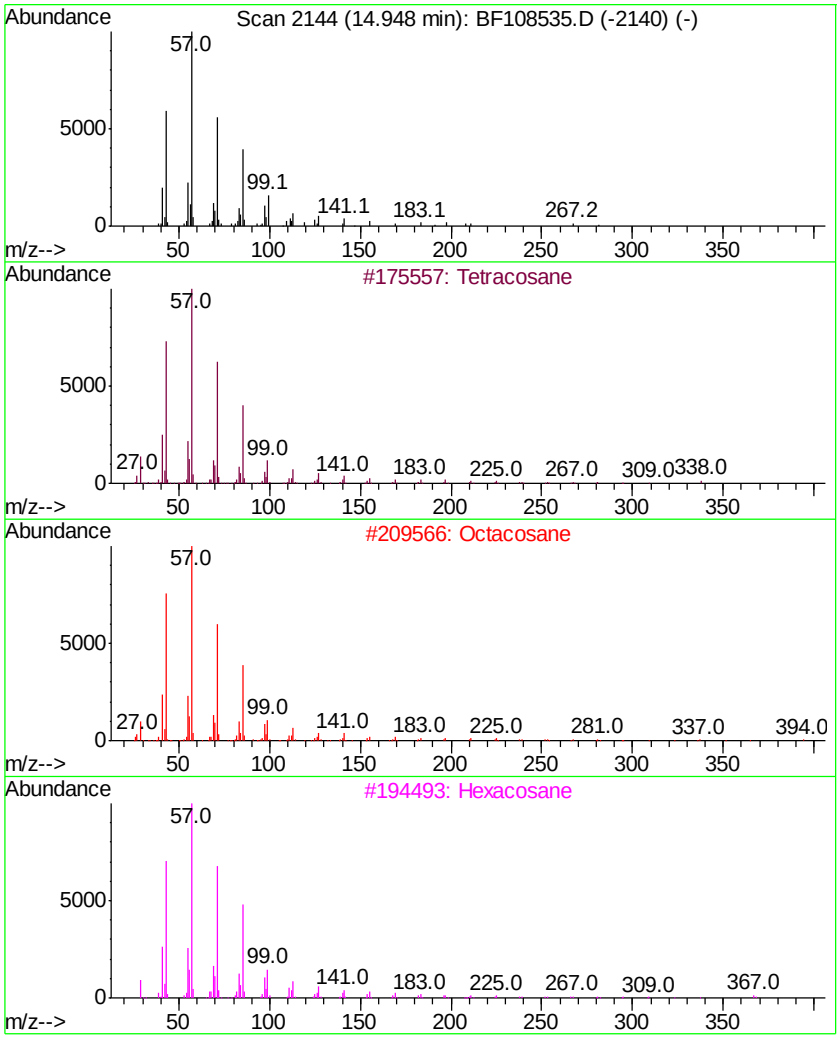
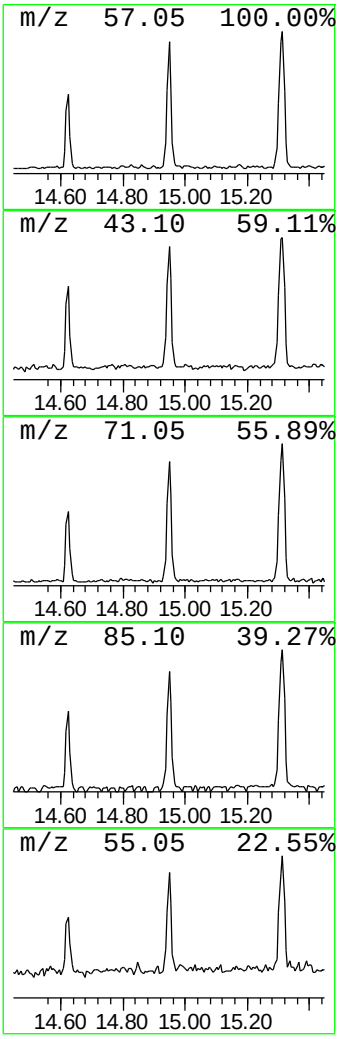
Peak Number 4 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	2.96 ng	104726	Chrysene-d12	14.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Hexatriacontane	507	C36H74	000630-06-8	91





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Sample : J4659-08
Misc :
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Instrument : BNA_F
ClientSampleId : 082218-SIDI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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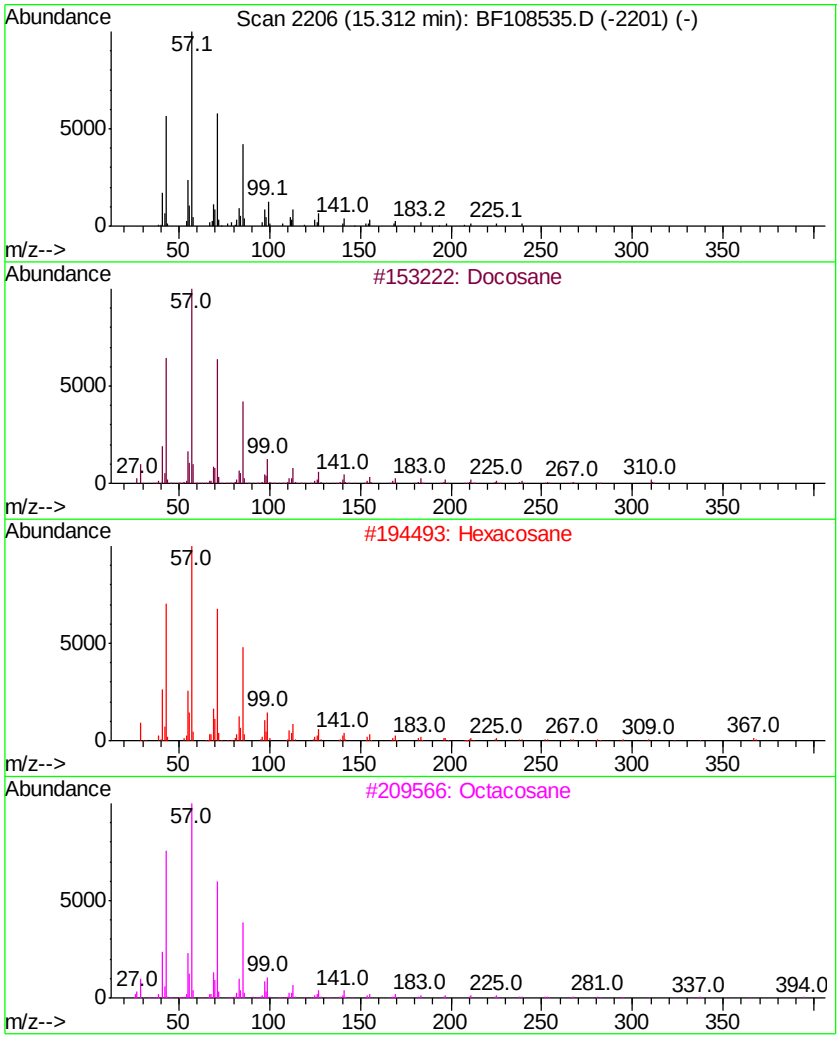
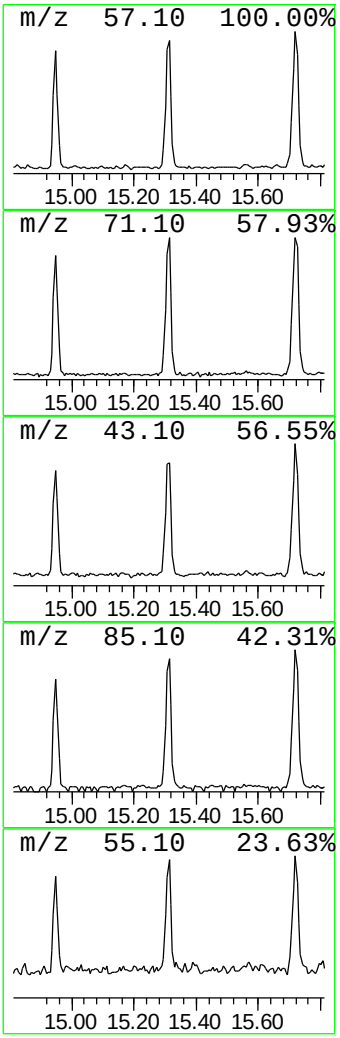
Peak Number 5 Docosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	4.28 ng	139419	Perylene-d12	15.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Heptacosane	380	C27H56	000593-49-7	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
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Misc :
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Instrument : BNA_F
ClientSampleId : 082218-SIDI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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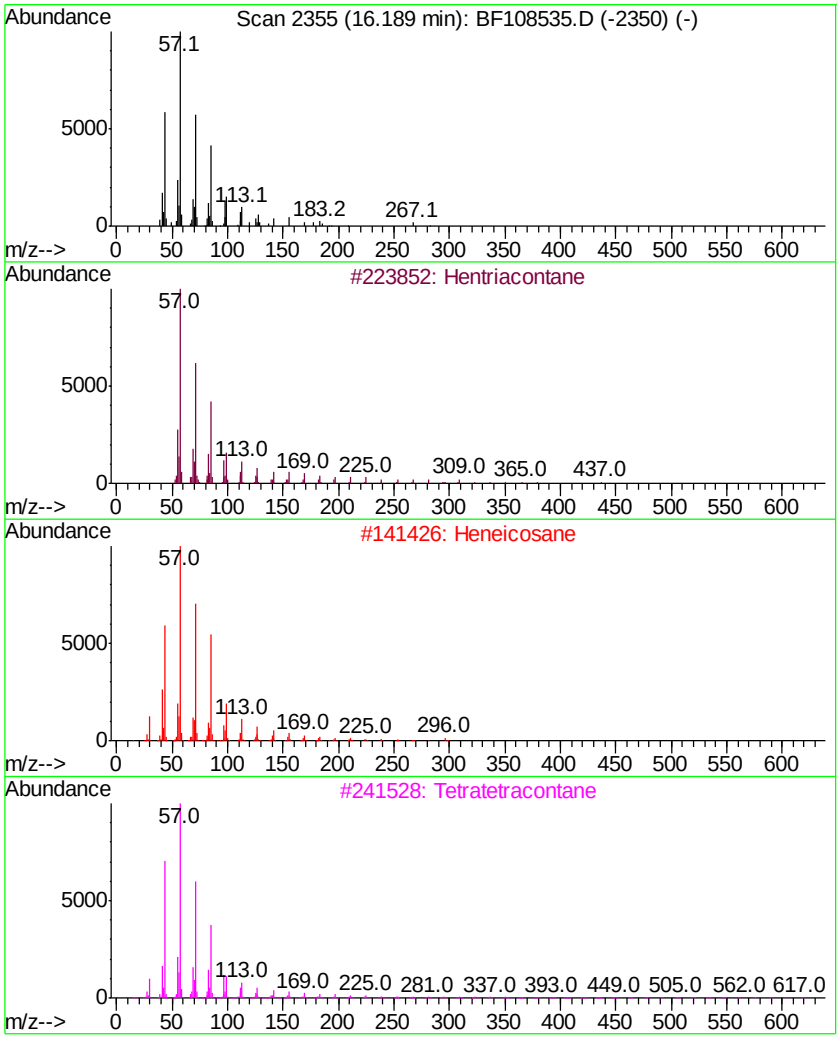
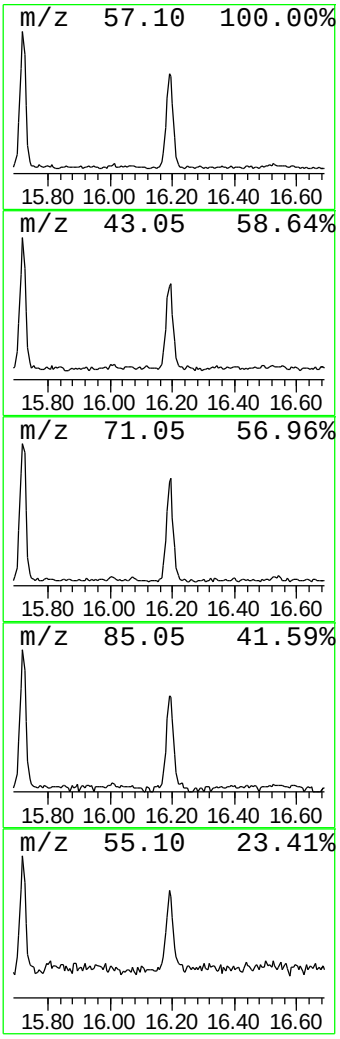
Peak Number 6 Hentriacontane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	4.30 ng	140127	Perylene-d12	15.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetratetracontane	619	C44H90	007098-22-8	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Octacosane	394	C28H58	000630-02-4	91





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Sample : J4659-08
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082218-SIDI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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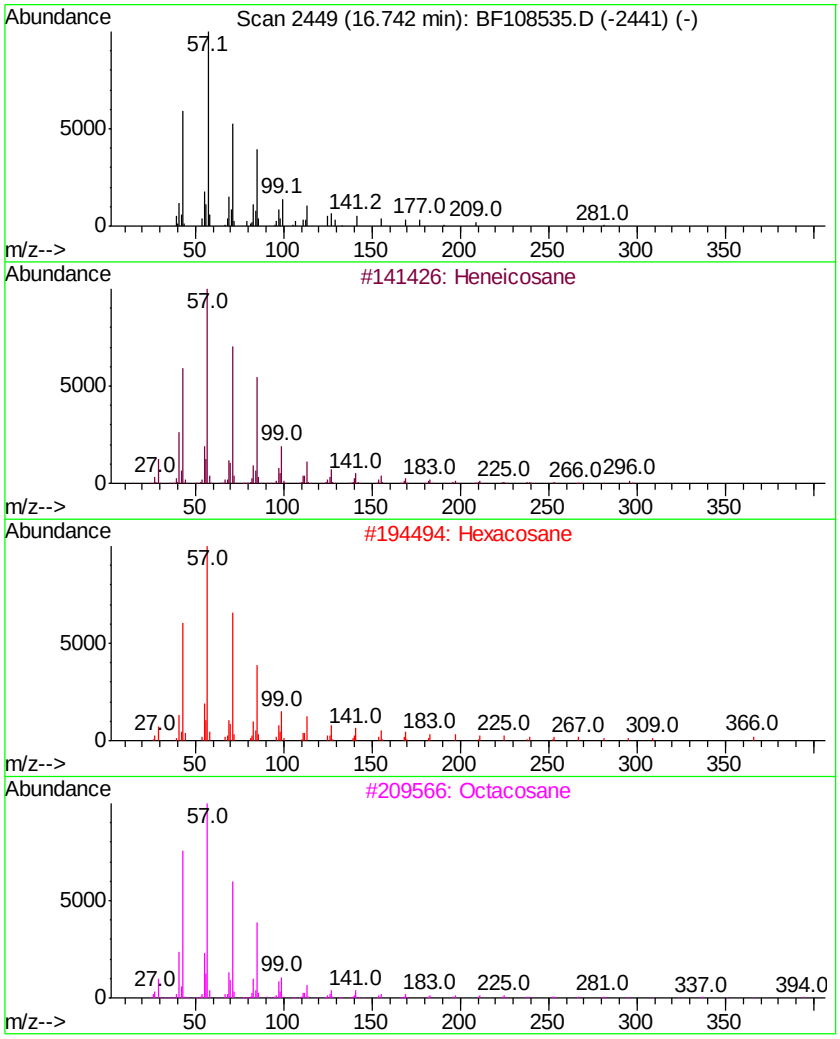
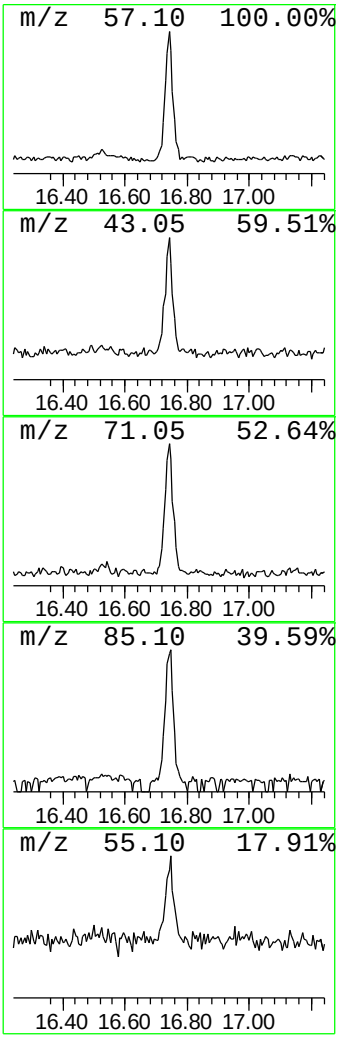
Peak Number 7 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.74	2.76 ng	90127	Perylene-d12	15.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Hexacosane	366	C26H54	000630-01-3	90
3	Octacosane	394	C28H58	000630-02-4	87
4	Hexadecane	226	C16H34	000544-76-3	87
5	Octadecane	254	C18H38	000593-45-3	87





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
unknown6.77	6.77	56.0	ng	1737030	1	7.00	620189	20.0
Triethyl citrate	10.70	2.4	ng	83609	3	10.04	712898	20.0
Tetracosane	14.95	3.0	ng	104726	5	14.19	707014	20.0
Docosane	15.31	4.3	ng	139419	6	15.74	652080	20.0
Hentriacontane	16.19	4.3	ng	140127	6	15.74	652080	20.0
Heneicosane	16.74	2.8	ng	90127	6	15.74	652080	20.0