LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM090518\
Data File : BM016679.D
Acq On : 05 Sep 2018 19:43
Operator : SJ/JU
Sample : J4741-23
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : A0C2-03-C

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_M\METHODS\8270-BM082118.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	5.516	375	379	392	rBV2	294300	537497	7.07%	1.993%
2	7.151	652	657	669	rBV	196630	394606	5.19%	1.463%
3	7.493	709	715	730	rBV2	831882	1419291	18.68%	5.262%
4	7.963	790	795	806	rBV2	235656	421681	5.55%	1.563%
5	8.281	842	849	863	rBV	963815	1595925	21.00%	5.917%
6	9.151	991	997	1010	rBV	551778	1010310	13.30%	3.746%
7	10.769	1266	1272	1280	rBV	258634	475681	6.26%	1.764%
8	13.222	1681	1689	1700	rBV	2238664	3121201	41.08%	11.572%
9	13.475	1724	1732	1739	rBV2	263170	412026	5.42%	1.528%
10	14.069	1828	1833	1841	rBV	349680	492576	6.48%	1.826%
11	14.604	1917	1924	1933	rBV2	411690	656867	8.65%	2.435%
12	15.698	2101	2110	2118	rBV4	89568	173057	2.28%	0.642%
13	16.104	2173	2179	2192	rBV	2357012	3481573	45.82%	12.908%
14	17.351	2384	2391	2406	rBV	625879	960649	12.64%	3.561%
15	18.210	2532	2537	2547	rBV2	240360	332962	4.38%	1.234%
16	19.474	2747	2752	2756	rBV5	90272	125021	1.65%	0.464%
17	19.945	2826	2832	2840	rBV	6698399	7598141	100.00%	28.169%
18	21.174	3038	3041	3049	rBV9	101409	211511	2.78%	0.784%
19	21.498	3092	3096	3104	rBV	1100879	1559912	20.53%	5.783%
20	22.615	3283	3286	3291	rVB	225968	281413	3.70%	1.043%
21	23.762	3476	3481	3491	rVB	857143	1711266	22.52%	6.344%

Sum of corrected areas: 26973166

LSC Report - Integrated Chromatogram

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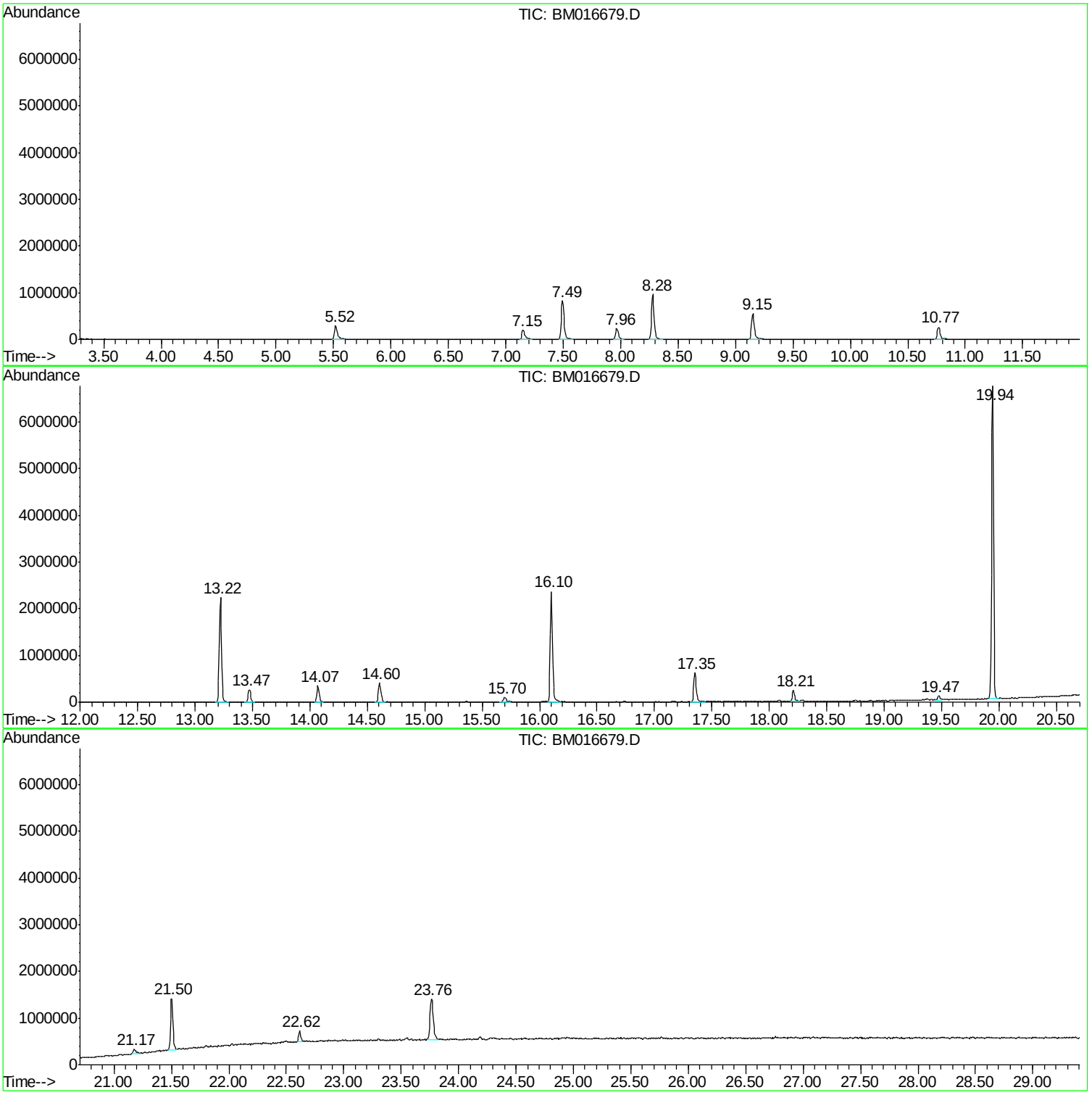
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : A0C2-03-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM090518\
Data File : BM016679.D
Acq On : 05 Sep 2018 19:43
Operator : SJ/JU
Sample : J4741-23
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : A0C2-03-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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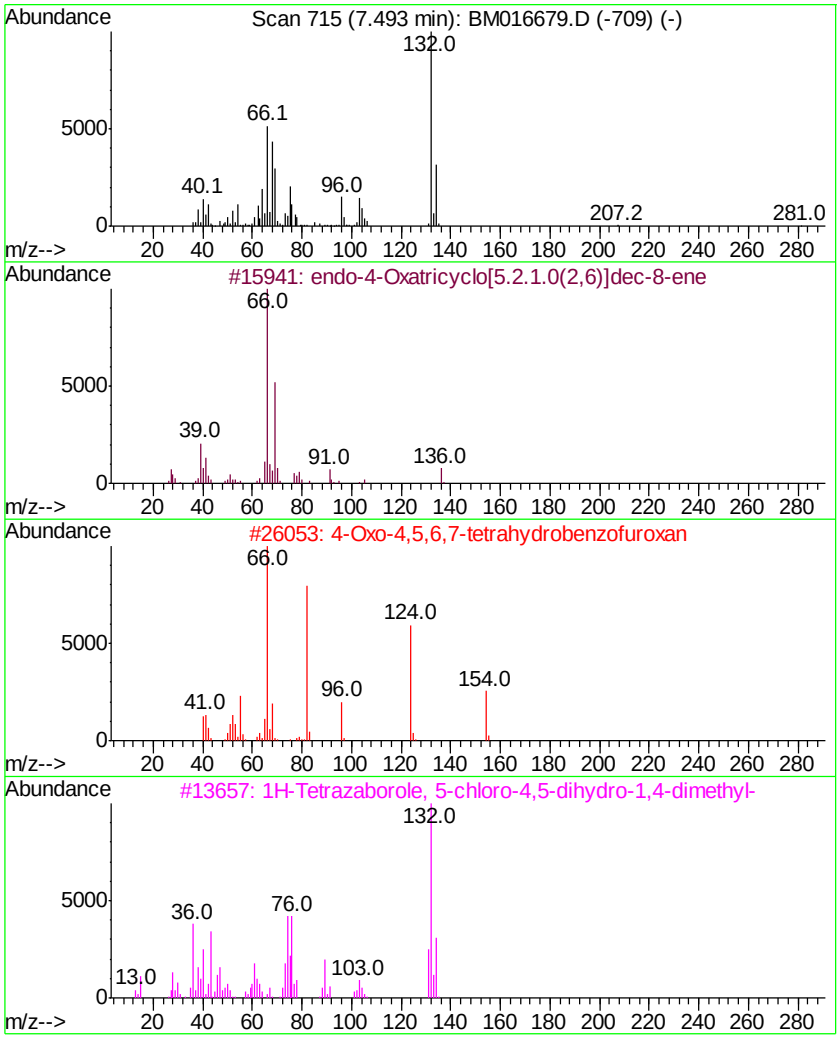
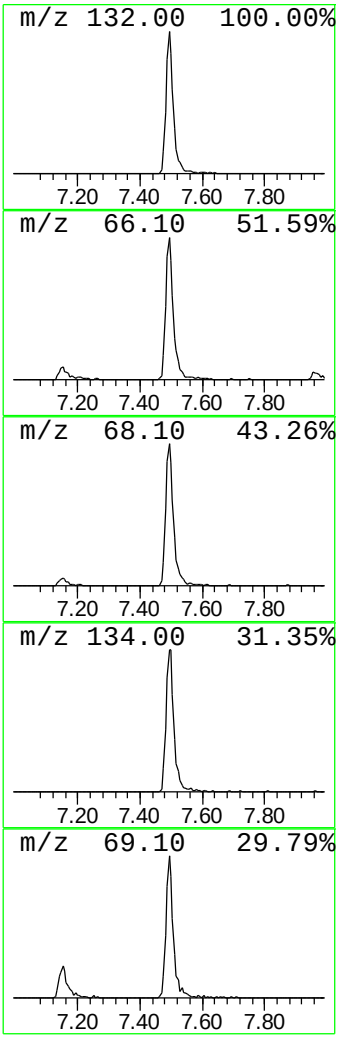
Peak Number 1 unknown7.49 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.49	67.32 ng	1419290	1,4-Dichlorobenzene-d4	7.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	endo-4-Oxatricyclo[5.2.1.0(2,6)]...	136	C9H12O	001528-23-0	27
2	4-Oxo-4,5,6,7-tetrahydrobenzofur...	154	C6H6N2O3	040345-49-1	25
3	1H-Tetrazaborole, 5-chloro-4,5-d...	132	C2H6BClN4	021960-49-6	22
4	1,4,4a,8a-Tetrahydro-1,4-methano...	174	C11H10O2	001200-89-1	16
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	14





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM090518\
Data File : BM016679.D
Acq On : 05 Sep 2018 19:43
Operator : SJ/JU
Sample : J4741-23
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : A0C2-03-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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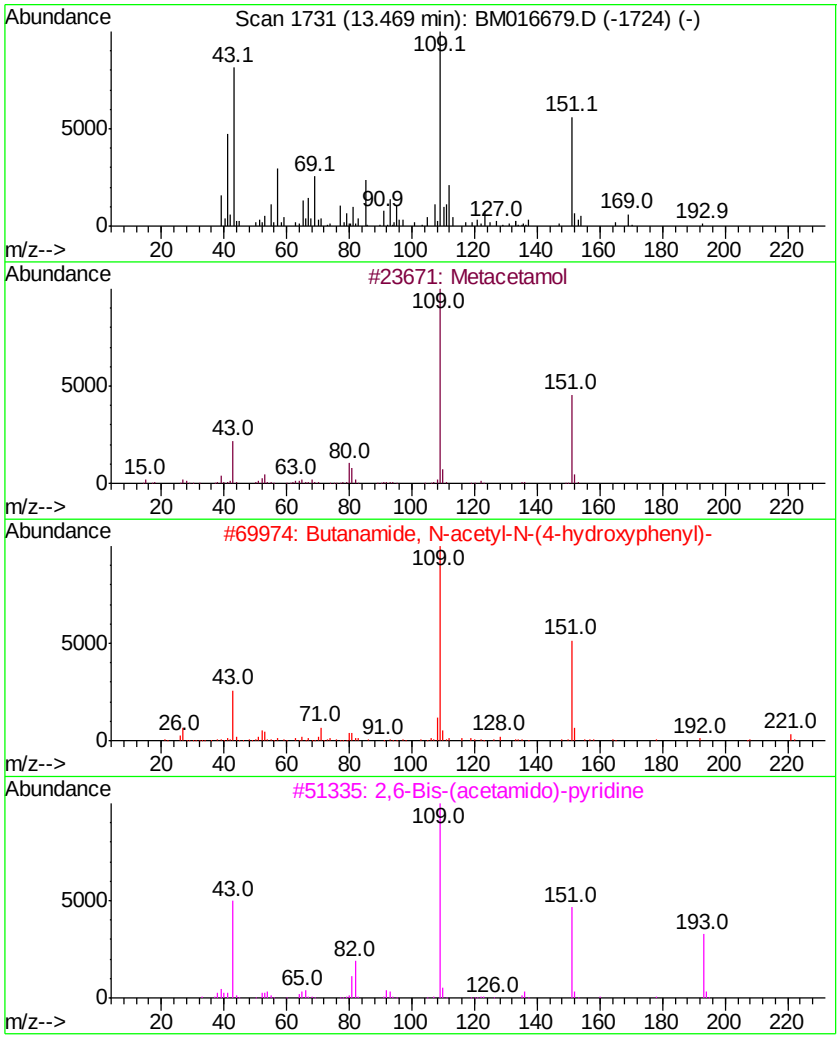
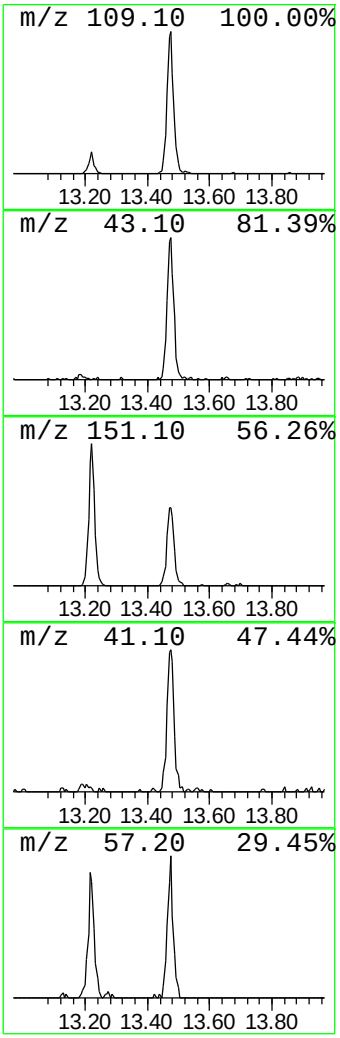
Peak Number 3 unknown13.47 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	12.55 ng	412026	Acenaphthene-d10	14.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Metacetamol	151	C8H9NO2	000621-42-1	49
2	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	47
3	2,6-Bis-(acetamido)-pyridine	193	C9H11N3O2	005441-02-1	47
4	N-Cyclopropyl-p-fluorobenzylamine	165	C10H12FN	1000250-88-9	38
5	Ethanone, 1-(1,3-dimethyl-3-cycl...	152	C10H16O	051733-68-7	35





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Data File : BM016679.D
Acq On : 05 Sep 2018 19:43
Operator : SJ/JU
Sample : J4741-23
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : A0C2-03-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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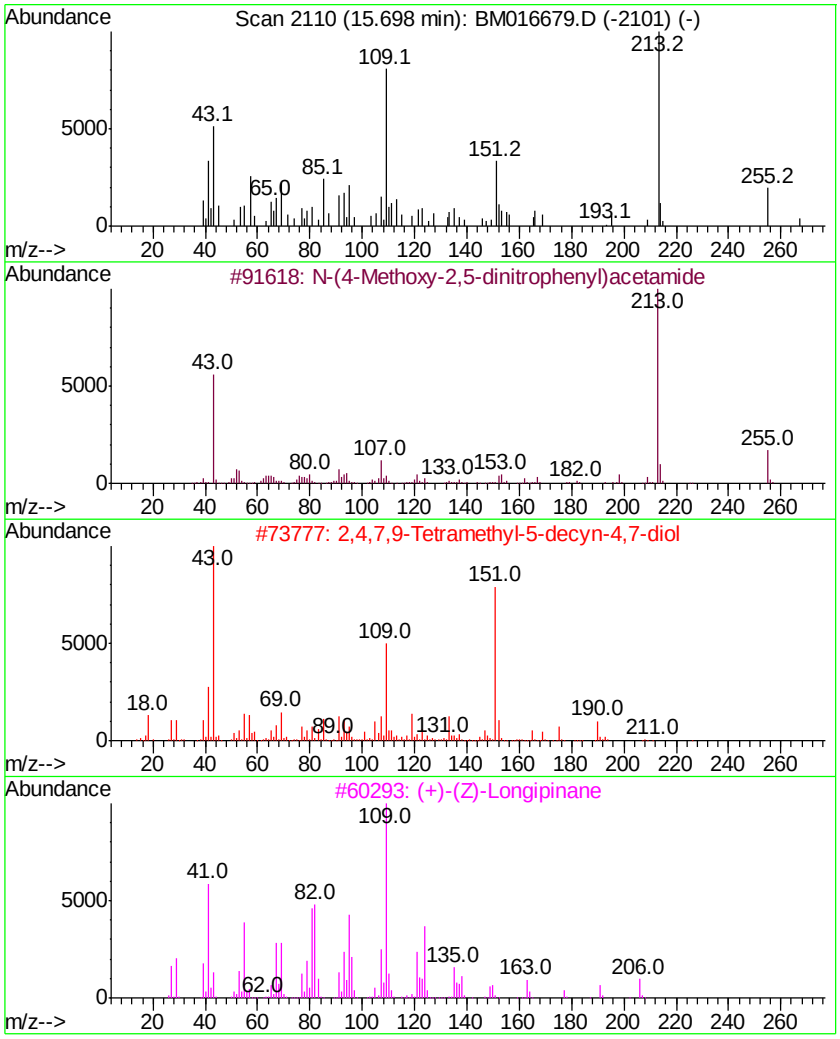
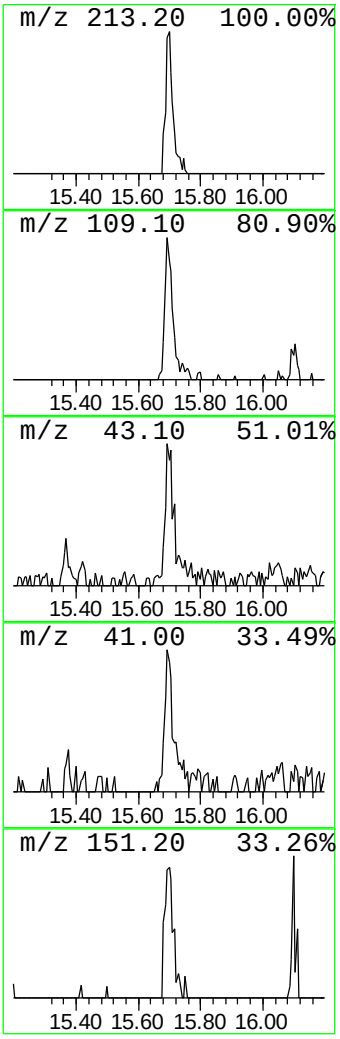
Peak Number 4 unknown15.70 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.70	5.27 ng	173057	Acenaphthene-d10	14.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-(4-Methoxy-2,5-dinitrophenyl)a...	255	C9H9N3O6	257932-05-1	38
2	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	27
3	(+)-(Z)-Longipinane	206	C15H26	1000156-12-3	27
4	Nitrobenzene, 3,4,5-trimethoxy-	213	C9H11NO5	006307-90-0	27
5	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	25





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM090518\
Data File : BM016679.D
Acq On : 05 Sep 2018 19:43
Operator : SJ/JU
Sample : J4741-23
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : A0C2-03-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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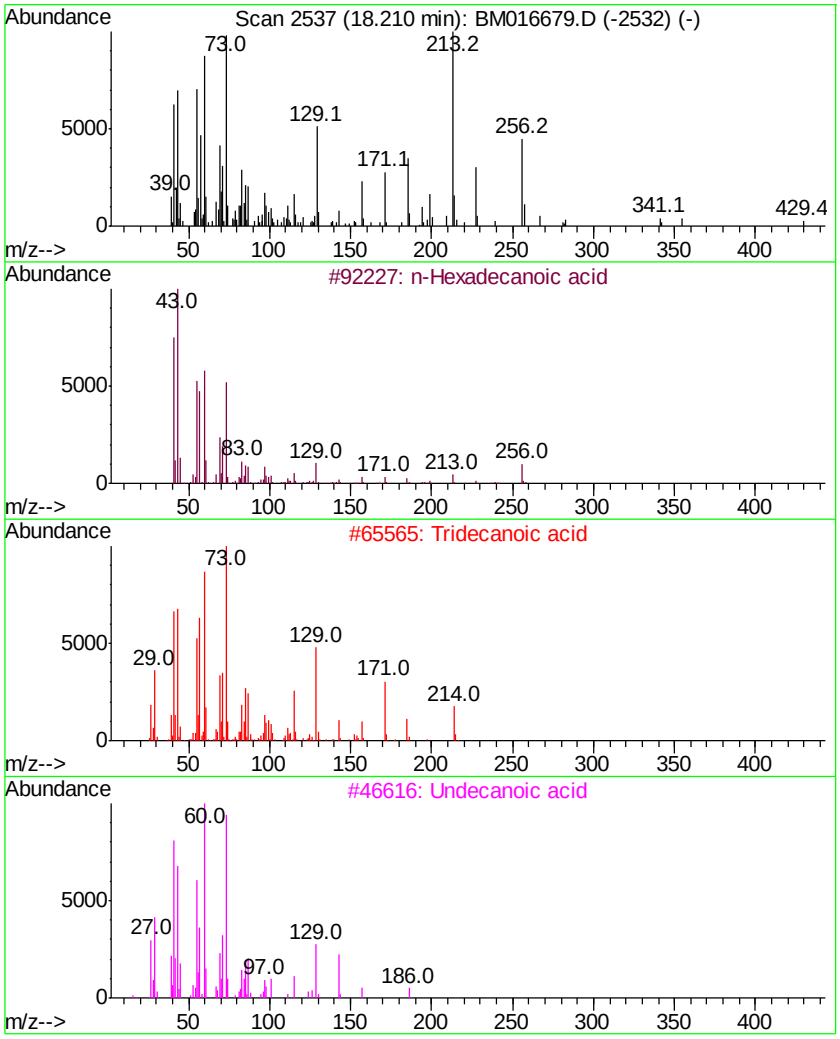
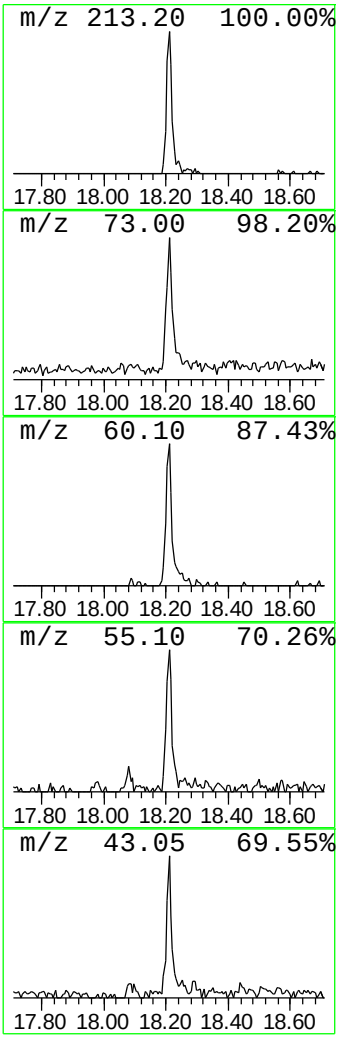
Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.21	6.93 ng	332962	Phenanthrene-d10	17.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Undecanoic acid	186	C11H22O2	000112-37-8	48
4	Thiazolo[4,5-d]pyrimidin-7(4H)-one	213	C7H7N3OS2	1000153-89-3	43
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	38





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Acq On : 05 Sep 2018 19:43
Operator : SJ/JU
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Misc :
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Instrument : BNA_M
ClientSampleId : A0C2-03-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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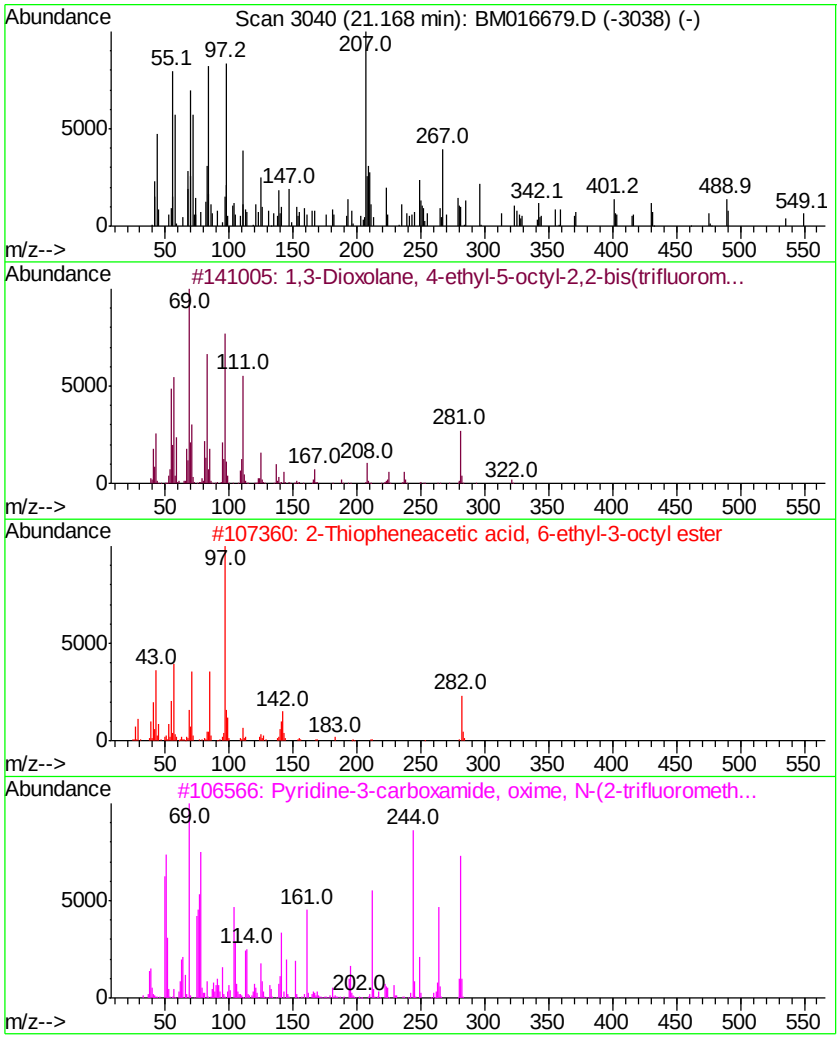
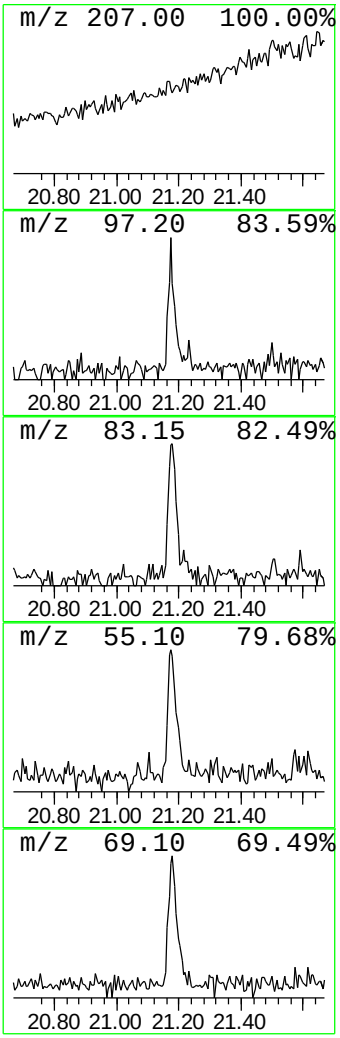
Peak Number 6 unknown21.17 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.17	2.71 ng	211511	Chrysene-d12	21.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 4-ethyl-5-octyl-2...	350	C15H24F6O2	038274-72-5	37
2	2-Thiopheneacetic acid, 6-ethyl-...	282	C16H26O2S	1000278-92-3	30
3	Pyridine-3-carboxamide, oxime, N...	281	C13H10F3N3O	288246-53-7	25
4	1,3-Dioxolane, 4-ethyl-5-octyl-2...	350	C15H24F6O2	038274-73-6	16
5	Cyclohexane, 1,1'-(2-propyl-1,3-...	250	C18H34	055030-21-2	12





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ClientSampleId : A0C2-03-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082118.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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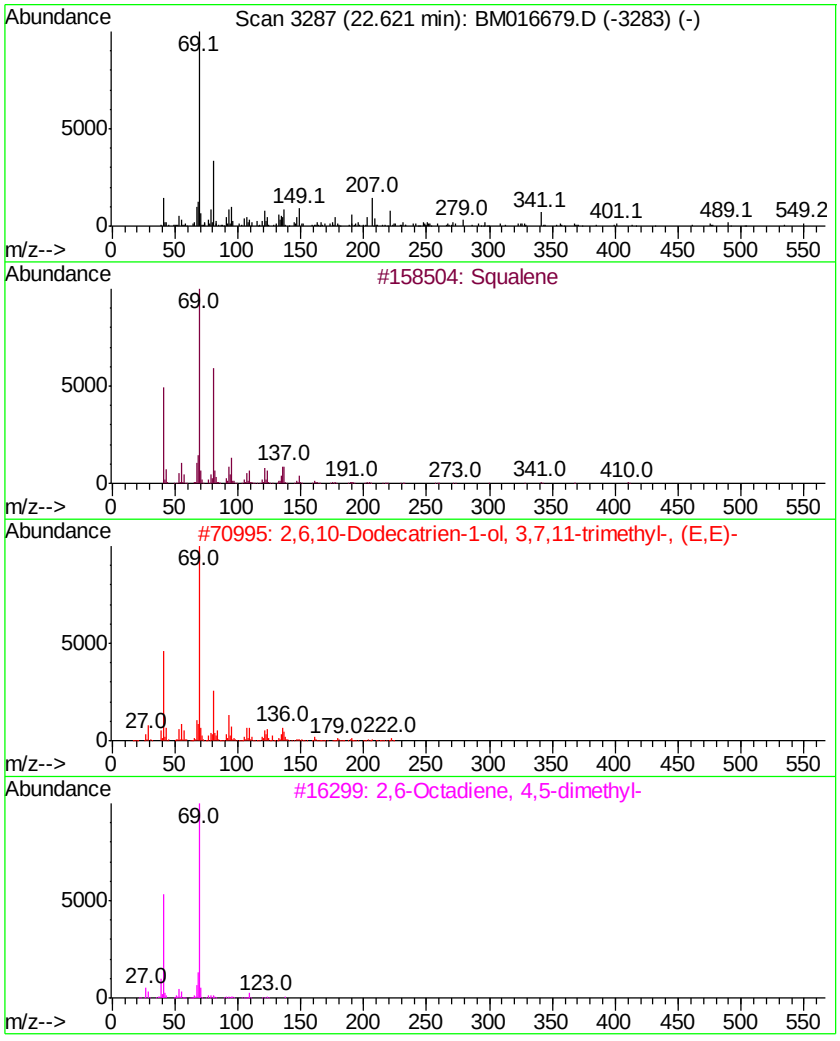
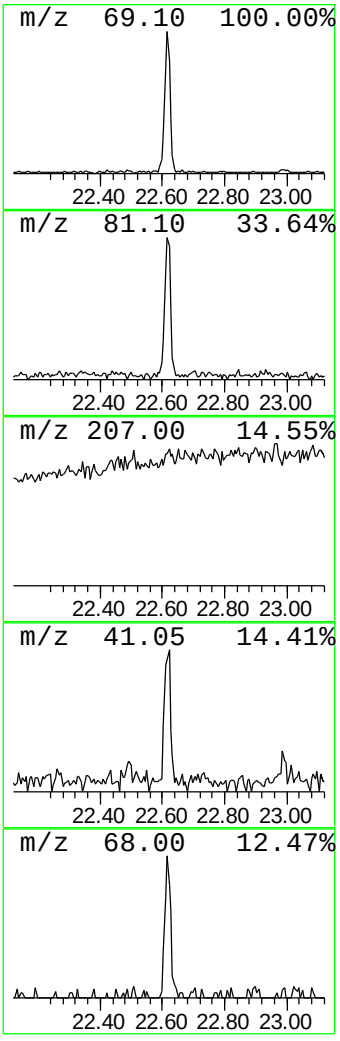
Peak Number 7 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.62	3.61 ng	281413	Chrysene-d12	21.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	64
2	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	000106-28-5	64
3	2,6-Octadiene, 4,5-dimethyl-	138	C10H18	018476-57-8	64
4	1,5-Heptadiene, 3,4-dimethyl-	124	C9H16	1000061-77-9	59
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown7.49	7.49	67.3	ng	1419290	1	7.97	421681	20.0
unknown13.47	13.47	12.6	ng	412026	3	14.60	656867	20.0
unknown15.70	15.70	5.3	ng	173057	3	14.60	656867	20.0
n-Hexadecanoic acid	18.21	6.9	ng	332962	4	17.35	960649	20.0
unknown21.17	21.17	2.7	ng	211511	5	21.50	1559910	20.0
Squalene	22.62	3.6	ng	281413	5	21.50	1559910	20.0