LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM102318\
Data File : BM017297.D
Acq On : 23 Oct 2018 22:42
Operator : MJ/SJ
Sample : J5604-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MS-VB-29736-BOX-2

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-BM101718.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	5.175	363	372	385	rBV	5451297	7645938	3.33%	2.023%
2	5.398	402	410	420	rVB	1481303	3067447	1.34%	0.812%
3	5.893	467	494	497	rBV2	41963368	229529716	100.00%	60.729%
4	6.845	649	656	665	rVB2	1422352	2641160	1.15%	0.699%
5	7.204	708	717	726	rBV	4296286	6666288	2.90%	1.764%
6	7.975	841	848	855	rVB	3721236	5930170	2.58%	1.569%
7	8.816	951	991	995	rBV2	8304459	47976262	20.90%	12.694%
8	10.433	1257	1266	1272	rBV	1613152	2732050	1.19%	0.723%
9	11.698	1472	1481	1489	rBV4	1076765	3083291	1.34%	0.816%
10	12.916	1681	1688	1694	rBV	7100271	10213755	4.45%	2.702%
11	13.263	1742	1747	1761	rVB	3752443	5907645	2.57%	1.563%
12	14.298	1918	1923	1930	rVB2	2016396	3106289	1.35%	0.822%
13	14.721	1989	1995	2003	rBV3	1656336	2955697	1.29%	0.782%
14	15.798	2171	2178	2183	rBV	5111466	7343556	3.20%	1.943%
15	15.851	2183	2187	2194	rVV	4332088	6049121	2.64%	1.600%
16	17.051	2386	2391	2398	rVB	2297793	3281016	1.43%	0.868%
17	17.909	2532	2537	2542	rVV	4597679	5870189	2.56%	1.553%
18	17.962	2542	2546	2553	rVB	1877816	2361053	1.03%	0.625%
19	19.592	2819	2823	2829	rVB	3354709	3836613	1.67%	1.015%
20	19.692	2834	2840	2845	rBV	8600386	10682172	4.65%	2.826%
21	21.244	3099	3104	3109	rBV	2736218	3501860	1.53%	0.927%
22	23.456	3474	3480	3493	rVB	1894217	3577358	1.56%	0.946%

Sum of corrected areas: 377958646

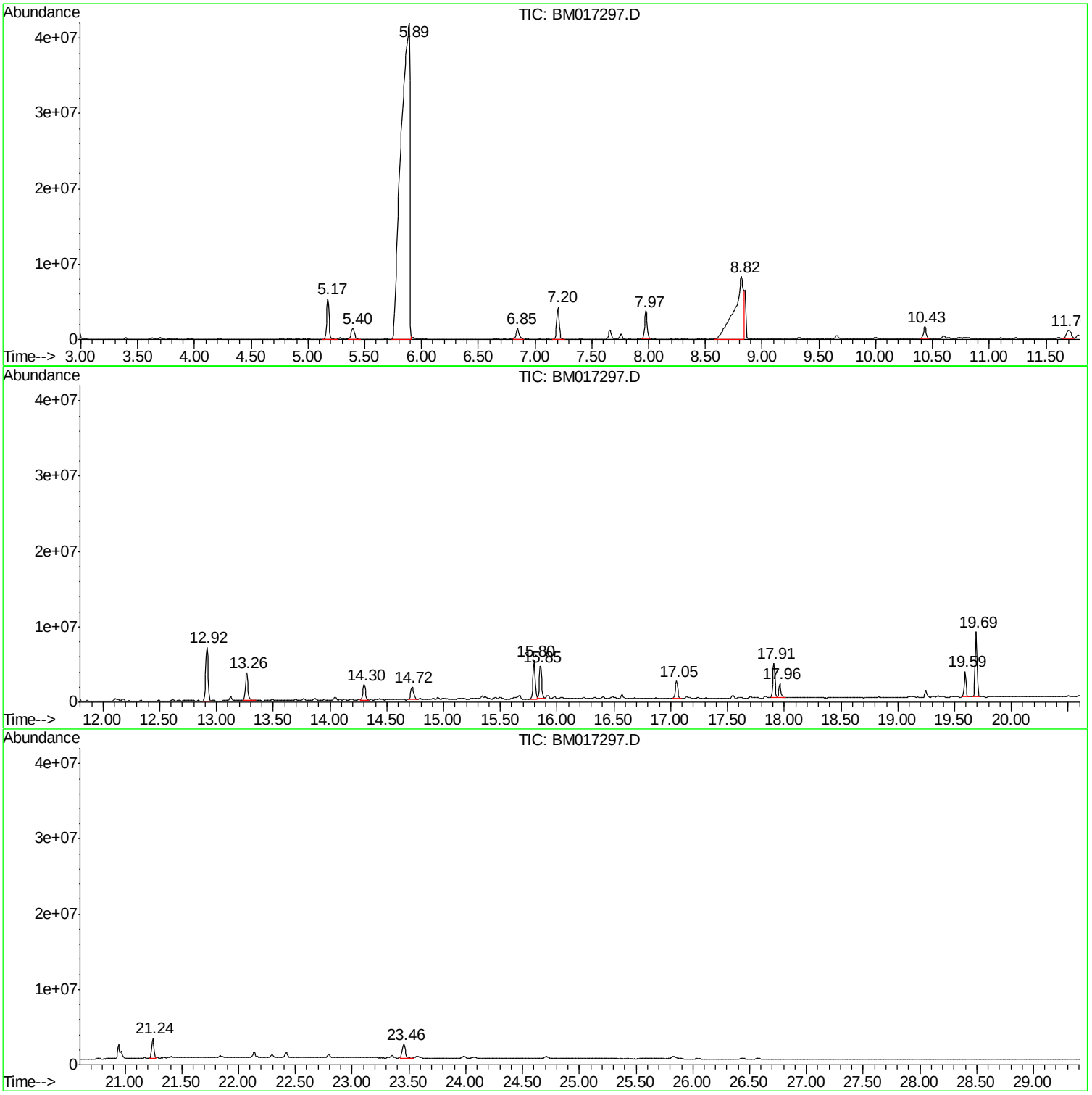
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM102318\
Data File : BM017297.D
Acq On : 23 Oct 2018 22:42
Operator : MJ/SJ
Sample : J5604-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MS-VB-29736-BOX-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM102318\
Data File : BM017297.D
Acq On : 23 Oct 2018 22:42
Operator : MJ/SJ
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ClientSampleId : MS-VB-29736-BOX-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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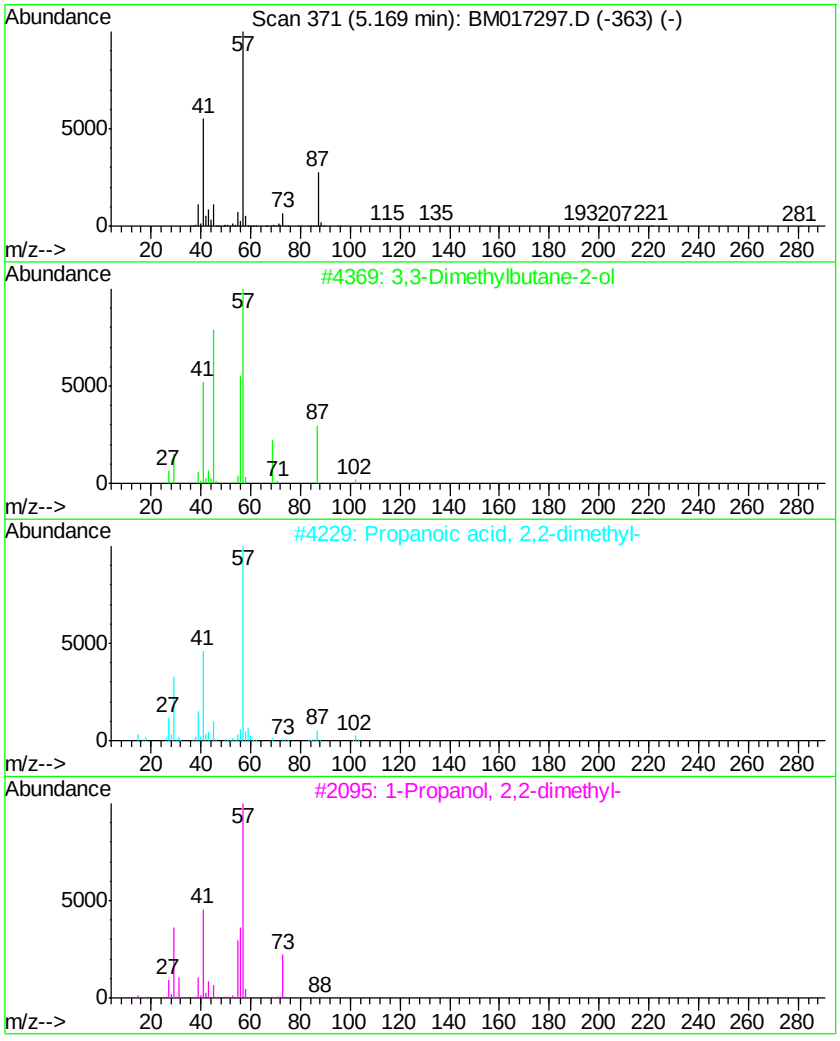
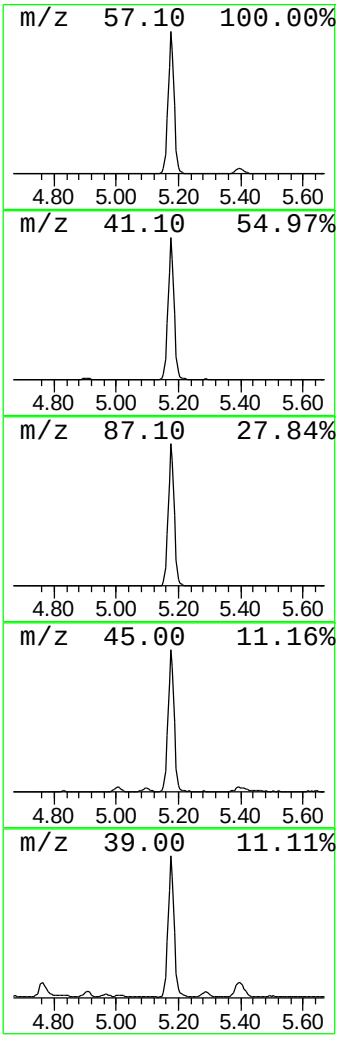
Peak Number 1 unknown5.17 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	25.79 ng	7645940	1,4-Dichlorobenzene-d4	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	45
2	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	38
3	1-Propanol, 2,2-dimethyl-	88	C5H12O	000075-84-3	25
4	Sulfurous acid, dibutyl ester	194	C8H18O3S	000626-85-7	25
5	1-Propanol, 2,2-dimethyl-, nitrate	133	C5H11NO3	000926-42-1	23





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Instrument : BNA_M
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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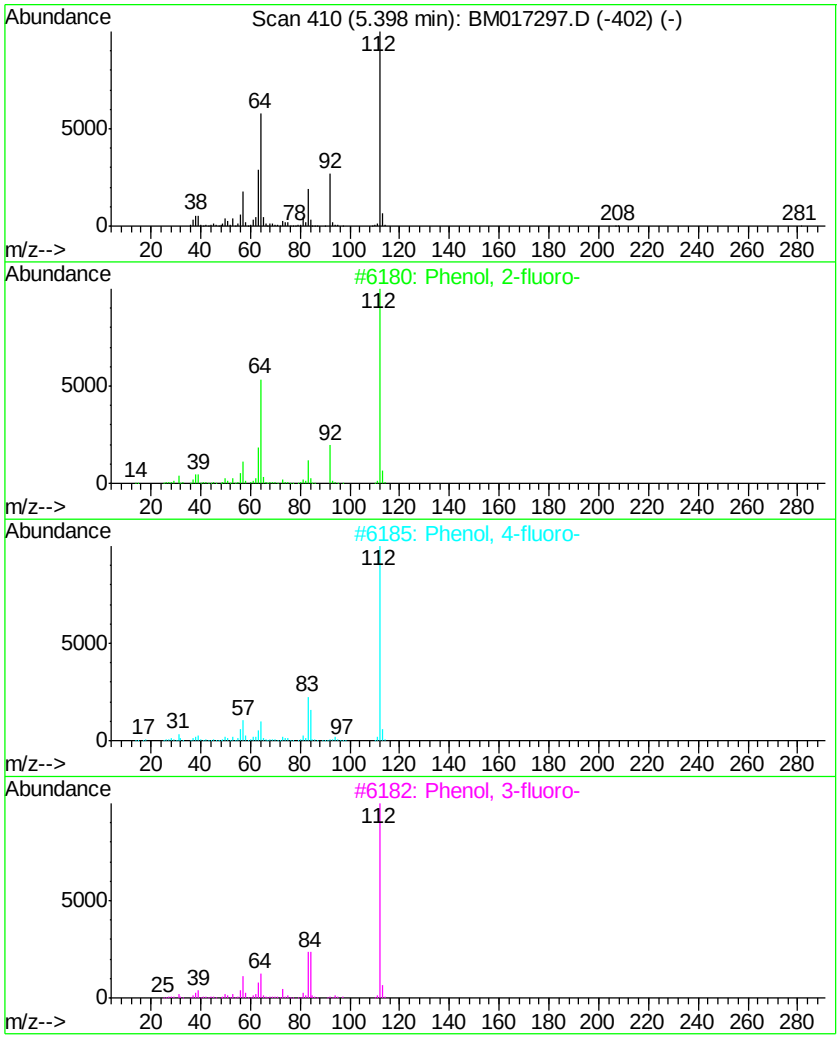
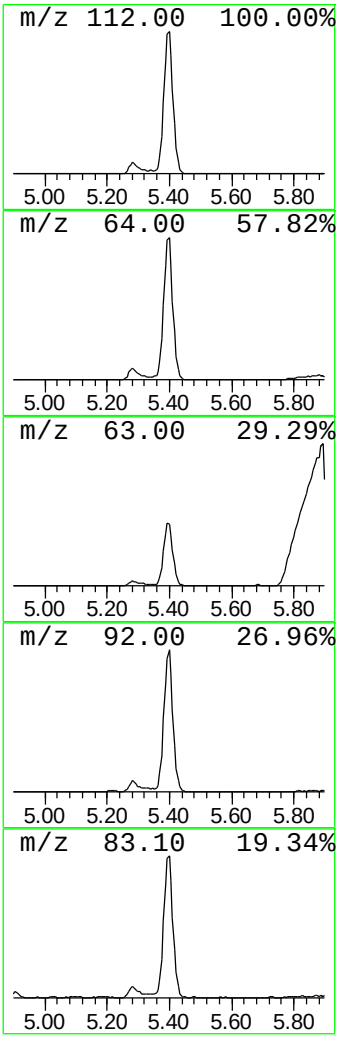
Peak Number 2 Phenol, 2-fluoro- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.40	10.35 ng	3067450	1,4-Dichlorobenzene-d4	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-fluoro-	112	C6H5FO	000367-12-4	90
2	Phenol, 4-fluoro-	112	C6H5FO	000371-41-5	30
3	Phenol, 3-fluoro-	112	C6H5FO	000372-20-3	12
4	1,4-Cyclohexanedione	112	C6H8O2	000637-88-7	10
5	Pyridine, 1,2,3,6-tetrahydro-1-n...	112	C5H8N2O	055556-92-8	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM102318\
Data File : BM017297.D
Acq On : 23 Oct 2018 22:42
Operator : MJ/SJ
Sample : J5604-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MS-VB-29736-BOX-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
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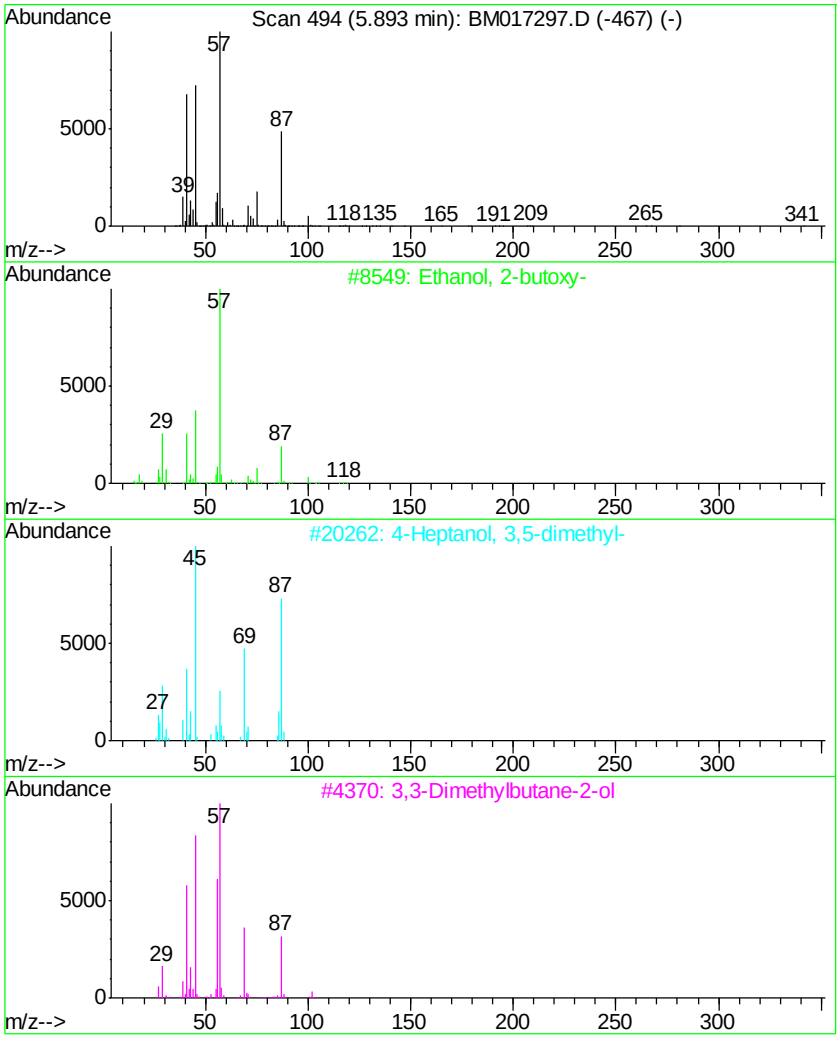
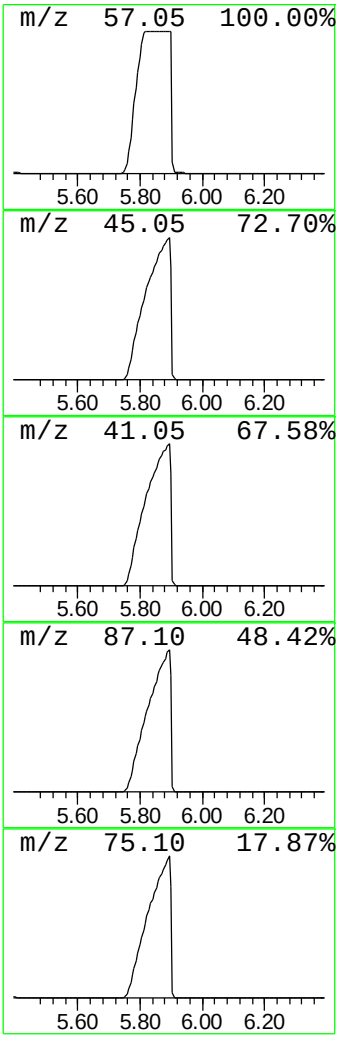
Peak Number 3 Ethanol, 2-butoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.89	774.11 ng	229530000	1,4-Dichlorobenzene-d4	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	64
2	4-Heptanol, 3,5-dimethyl-	144	C9H20O	019549-79-2	50
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	47
4	4,5-Octanediol, 3,6-dimethyl-	174	C10H22O2	1000153-21-1	38
5	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	38





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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MS-VB-29736-BOX-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
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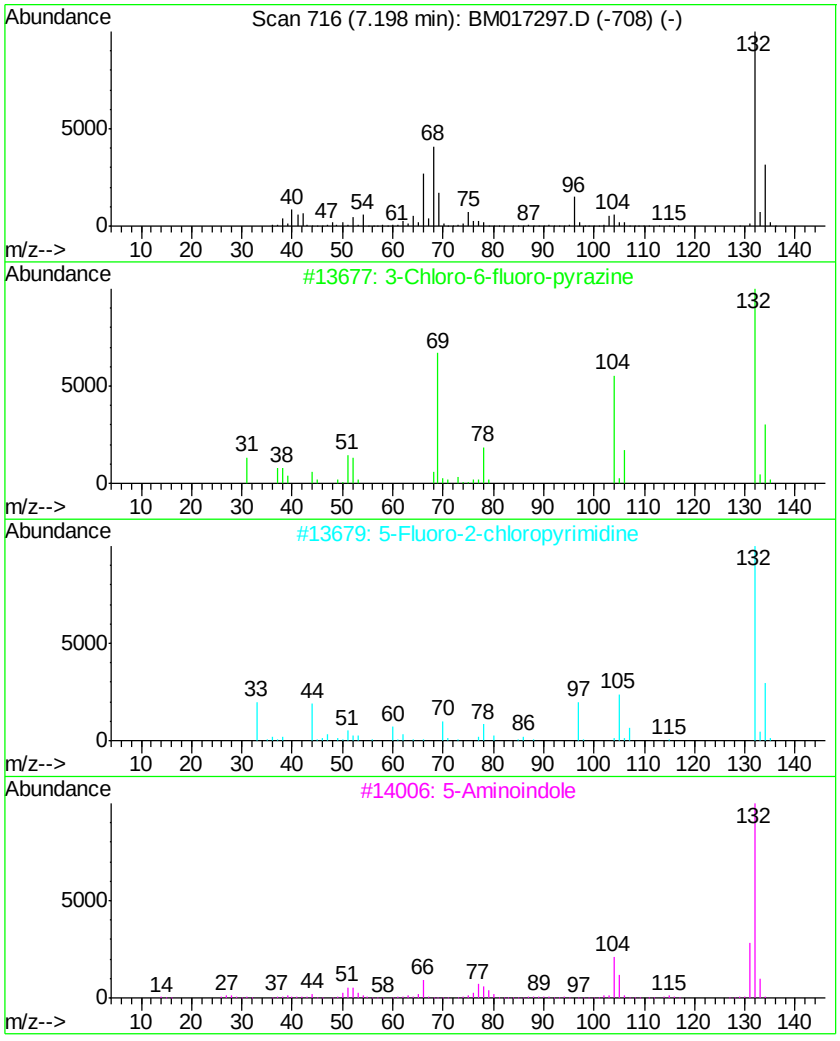
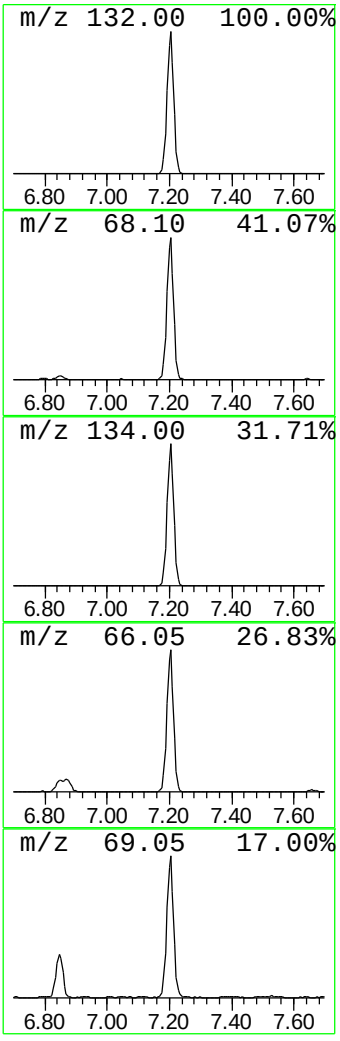
****

Peak Number 4 unknown7.20 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	22.48 ng	6666290	1,4-Dichlorobenzene-d4	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

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Data File : BM017297.D
Acq On : 23 Oct 2018 22:42
Operator : MJ/SJ
Sample : J5604-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MS-VB-29736-BOX-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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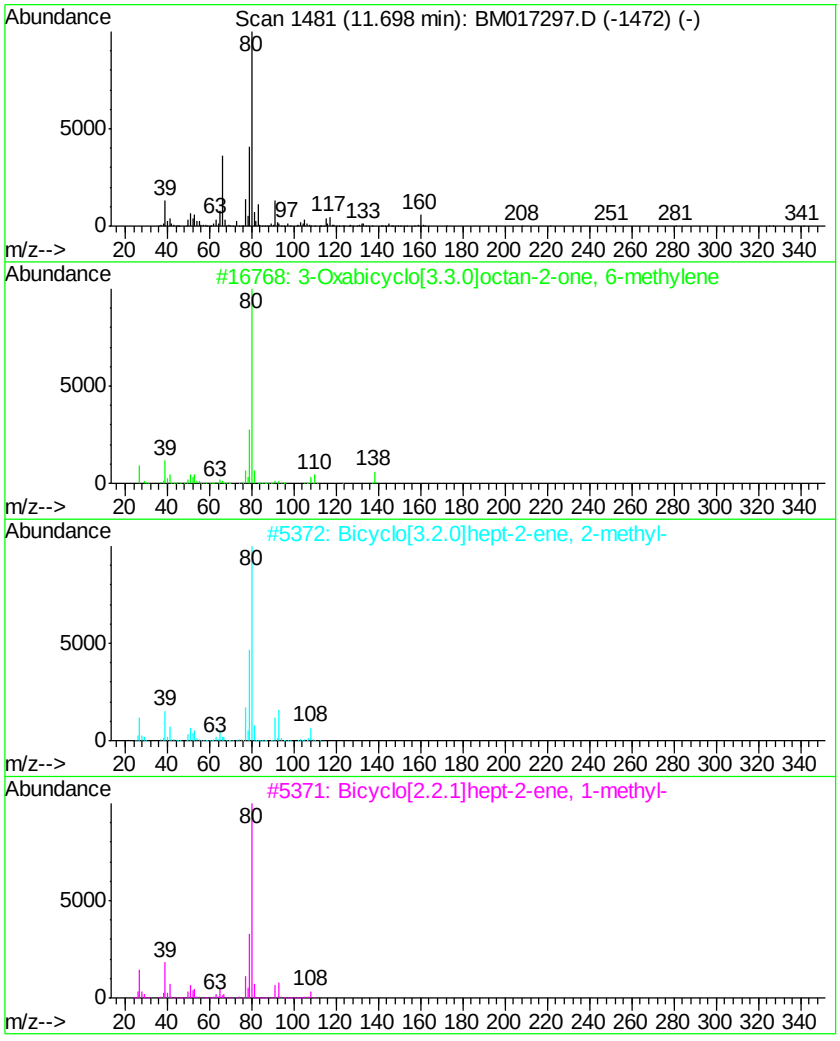
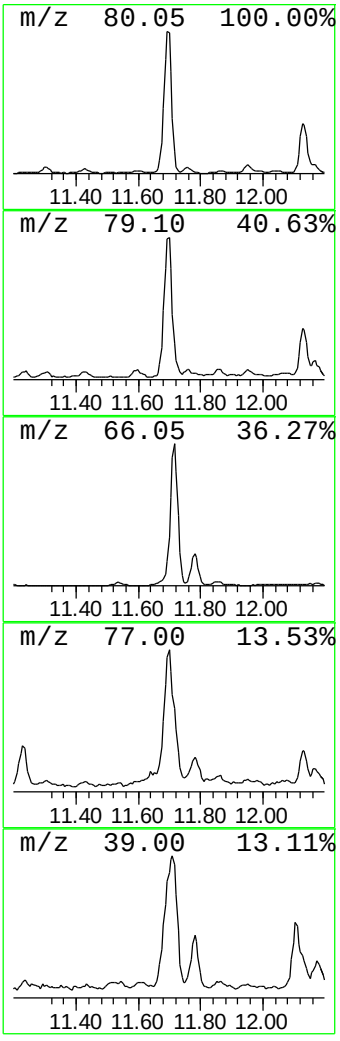
****

Peak Number 6 3-Oxabicyclo[3.3.0]octan-2-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	22.57 ng	3083290	Naphthalene-d8	10.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Oxabicyclo[3.3.0]octan-2-one, ...	138	C8H10O2	1000152-82-0	59
2	Bicyclo[3.2.0]hept-2-ene, 2-methyl-	108	C8H12	094122-58-4	59
3	Bicyclo[2.2.1]hept-2-ene, 1-methyl-	108	C8H12	000822-73-1	59
4	Bicyclo[2.2.2]oct-2-ene	108	C8H12	000931-64-6	59
5	Bicyclo[2.2.1]hept-2-ene, 2-methyl-	108	C8H12	000694-92-8	59





Library Search Compound Report

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Data File : BM017297.D
Acq On : 23 Oct 2018 22:42
Operator : MJ/SJ
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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-VB-29736-BOX-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
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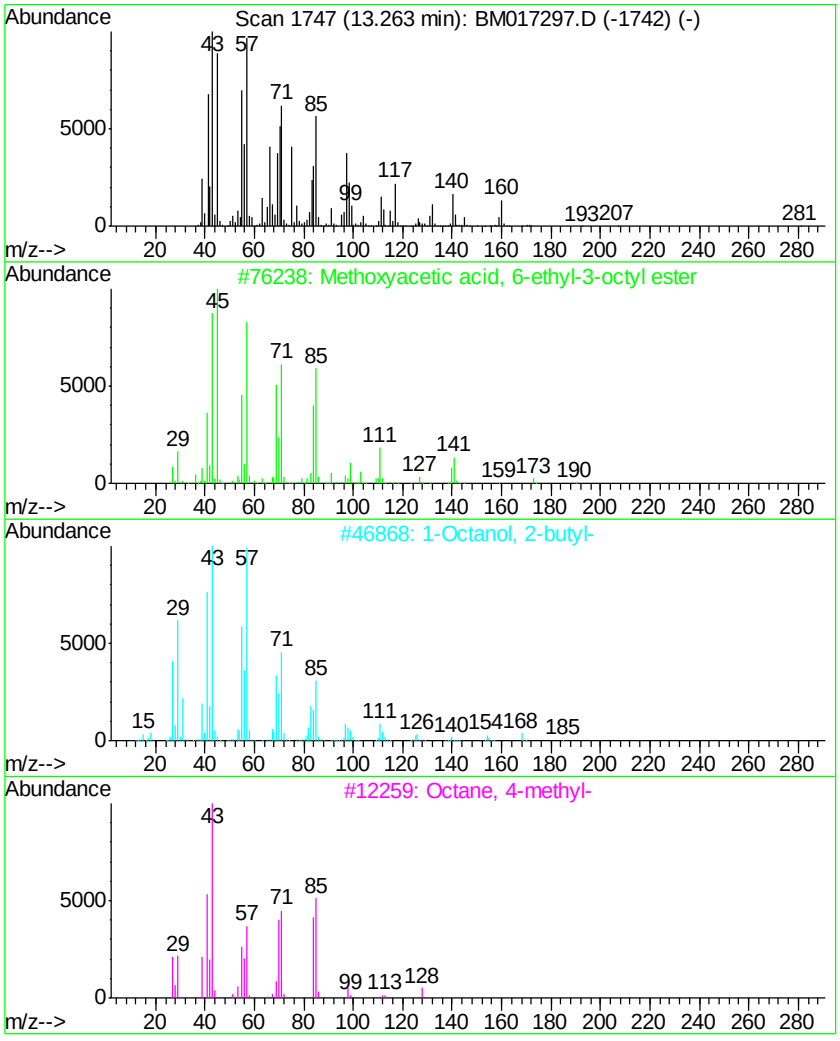
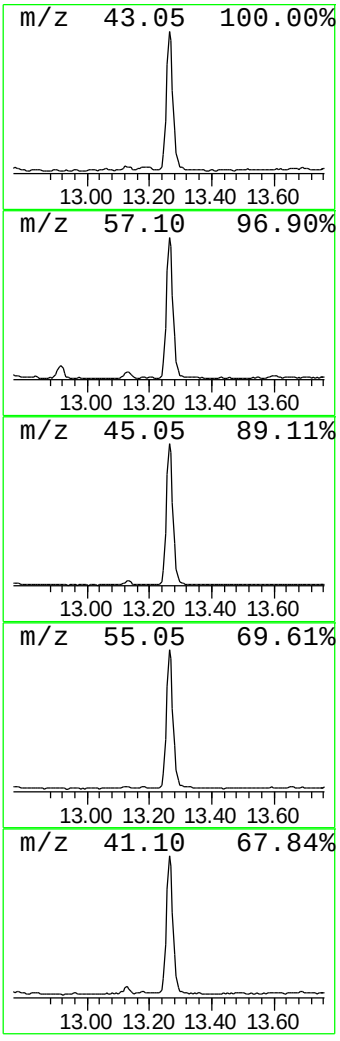
****

Peak Number 7 unknown13.26 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.26	38.04 ng	5907650	Acenaphthene-d10	14.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methoxyacetic acid, 6-ethyl-3-oc...	230	C13H26O3	1000282-69-8	27
2	1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	14
3	Octane, 4-methyl-	128	C9H20	002216-34-4	14
4	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	11
5	Undecane, 3,7-dimethyl-	184	C13H28	017301-29-0	10





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Instrument : BNA_M
ClientSampleId : MS-VB-29736-BOX-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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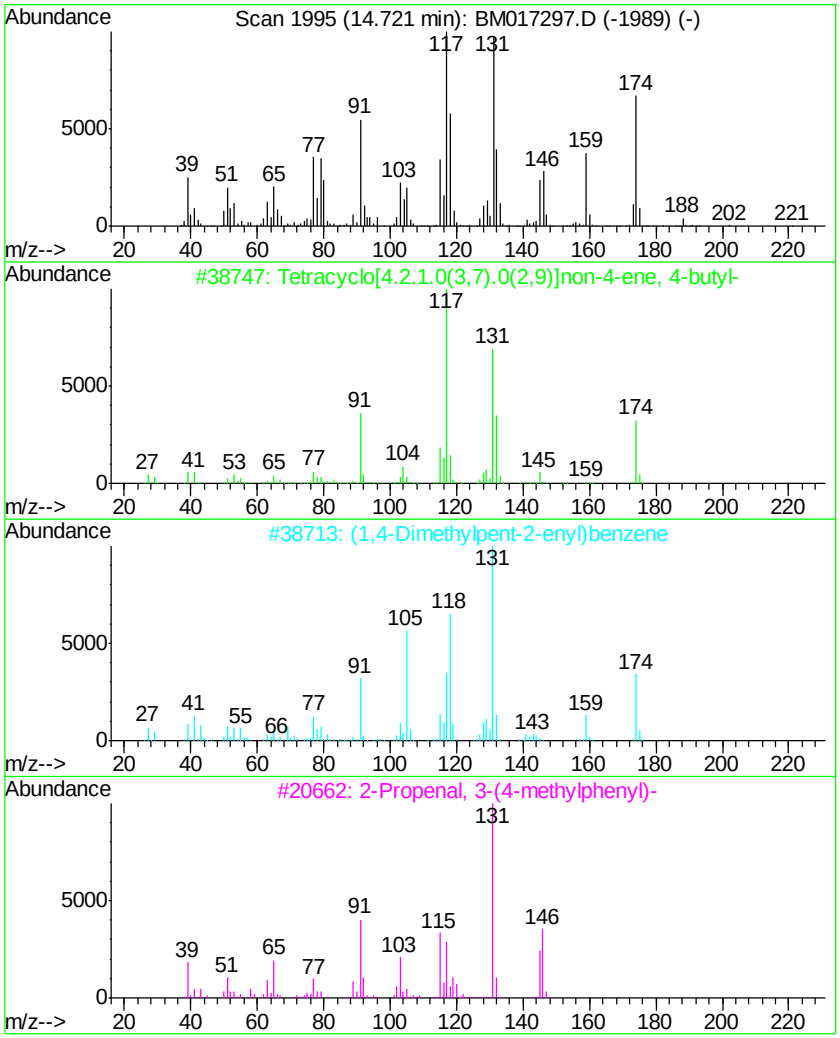
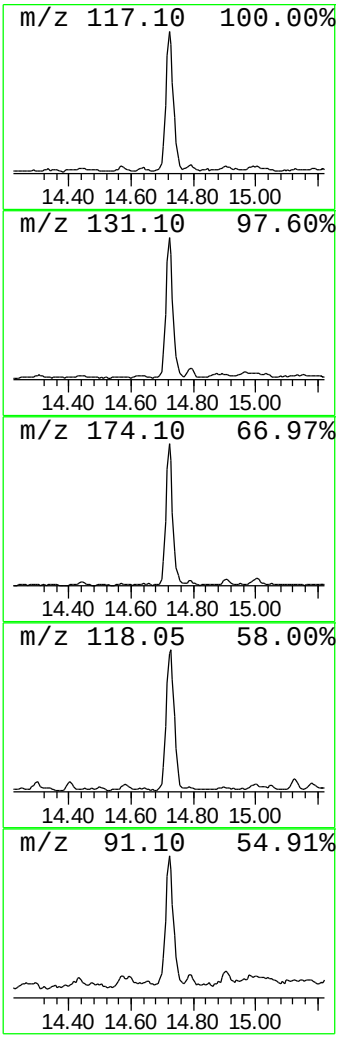
****

Peak Number 8 Tetracyclo[4.2.1.0(3,7).0(2... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	19.03 ng	2955700	Acenaphthene-d10	14.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracyclo[4.2.1.0(3,7).0(2,9)]n...	174	C13H18	1000164-31-2	64
2	(1,4-Dimethylpent-2-enyl)benzene	174	C13H18	1000184-97-9	49
3	2-Propenal, 3-(4-methylphenyl)-	146	C10H10O	001504-75-2	46
4	Pentacyclo[5.2.1.0(1,5).0(5,9).0...	132	C10H12	1000185-59-0	45
5	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	42





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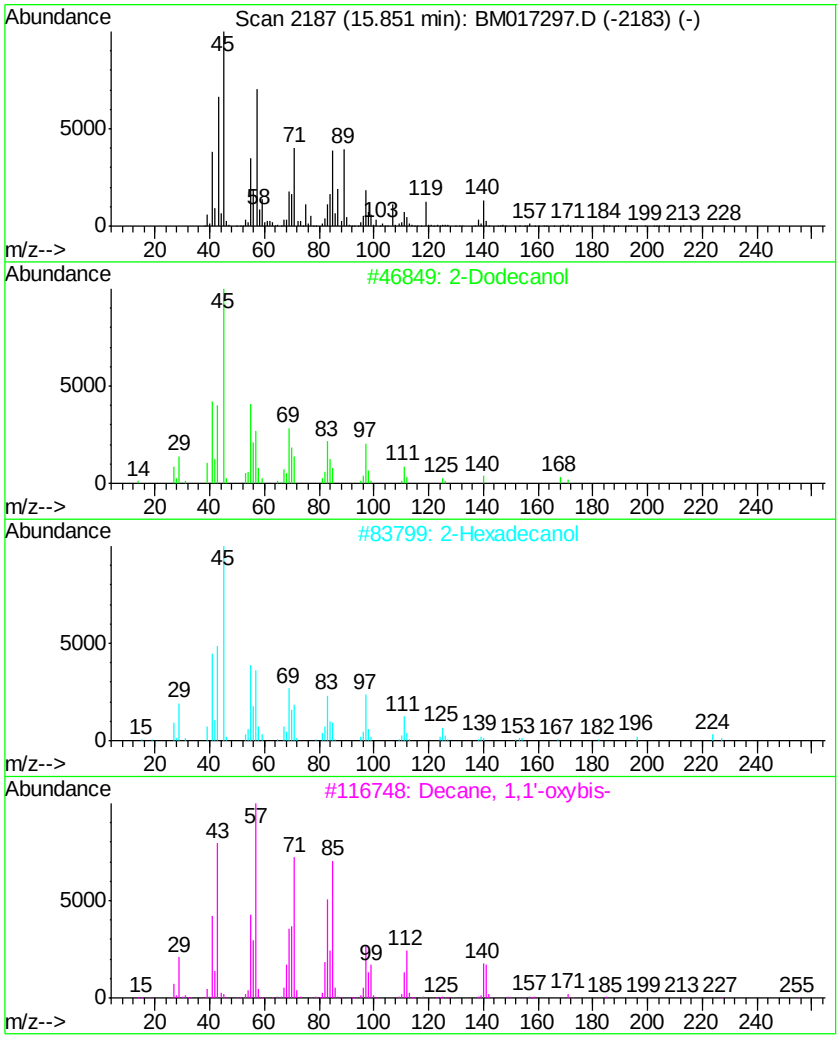
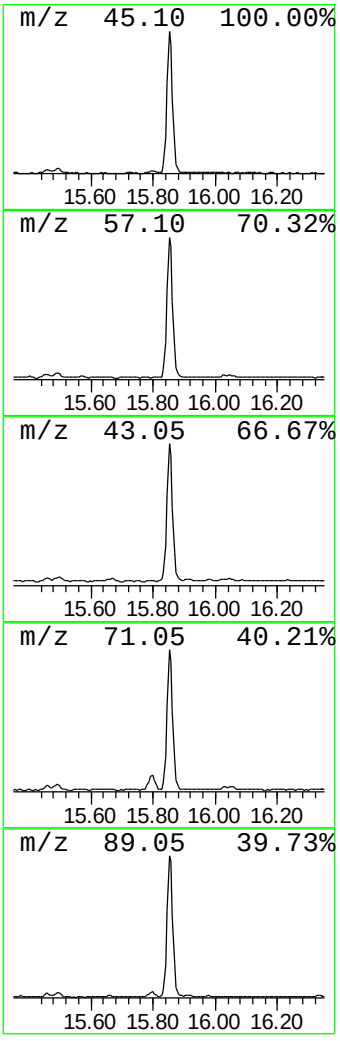
****

Peak Number 9 unknown15.85 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.85	36.87 ng	6049120	Phenanthrene-d10	17.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Dodecanol	186	C12H26O	010203-28-8	35
2	2-Hexadecanol	242	C16H34O	014852-31-4	35
3	Decane, 1,1'-oxybis-	298	C20H42O	002456-28-2	30
4	Propanoic acid, 2-methyl-, decyl...	228	C14H28O2	005454-22-8	25
5	Undecane, 4,7-dimethyl-	184	C13H28	017301-32-5	22





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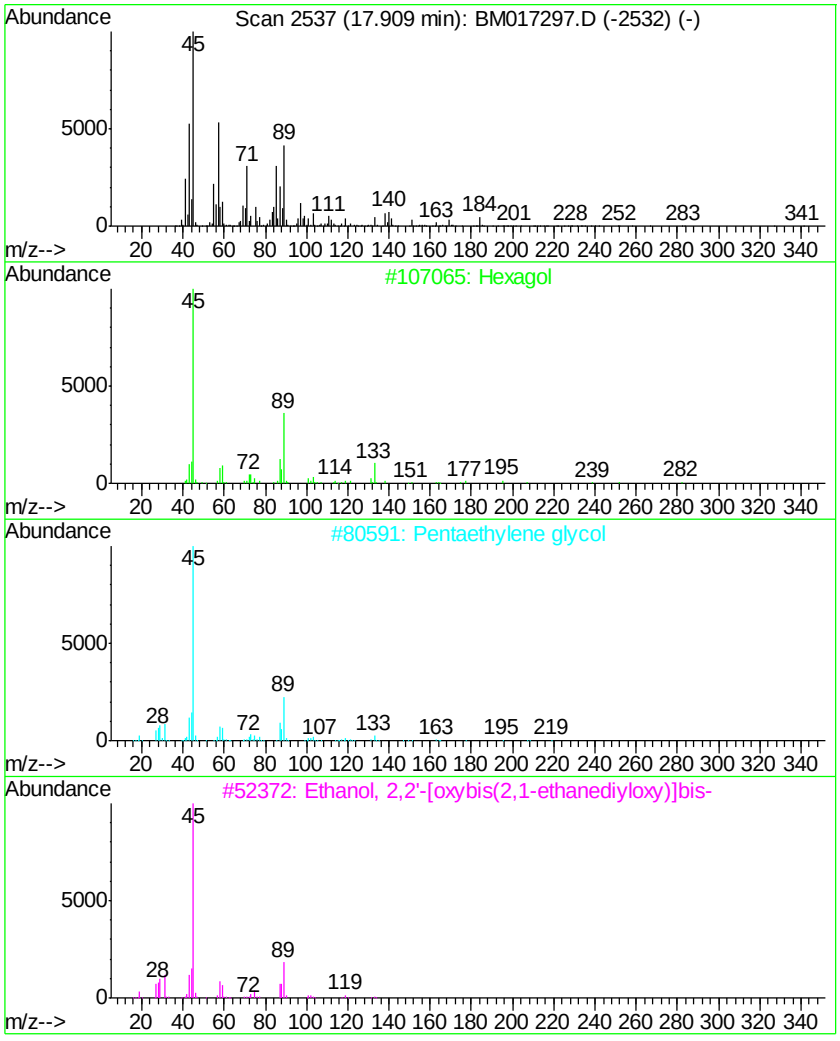
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

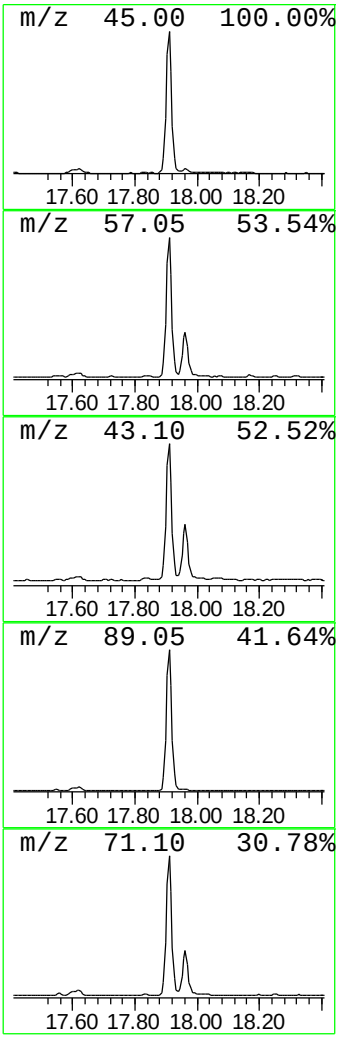
****

Peak Number 10 Hexagol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.91	35.78 ng	5870190	Phenanthrene-d10	17.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexagol	282	C12H26O7	002615-15-8	62
2	Pentaethylene glycol	238	C10H22O6	004792-15-8	50
3	Ethanol, 2,2'-[oxybis(2,1-ethane...	194	C8H18O5	000112-60-7	43
4	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	38
5	Diisopropyl ether	102	C6H14O	000108-20-3	38





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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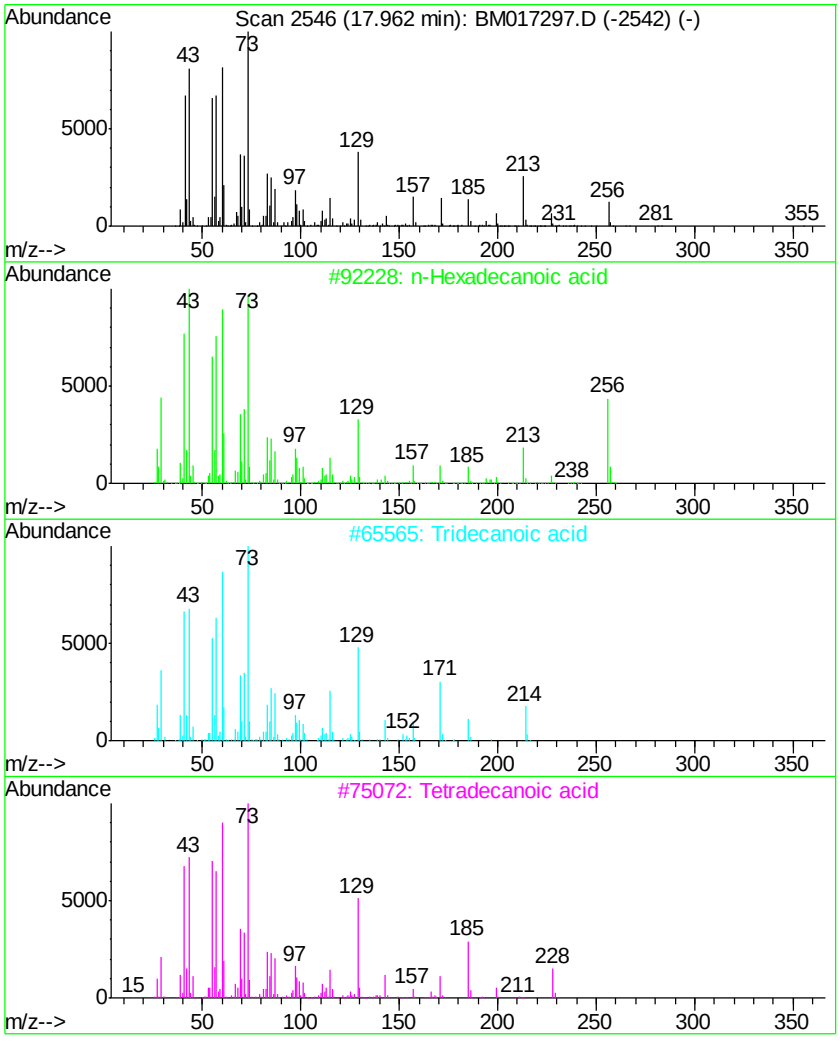
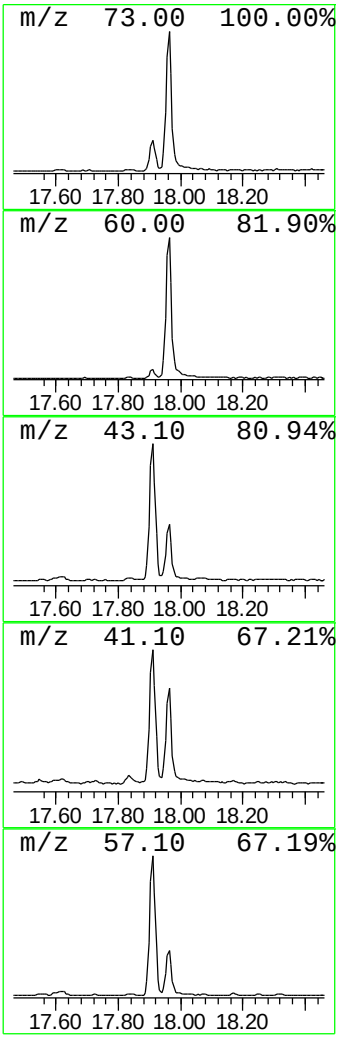
Peak Number 11 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.96	14.39 ng	2361050	Phenanthrene-d10	17.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM102318\
Data File : BM017297.D
Acq On : 23 Oct 2018 22:42
Operator : MJ/SJ
Sample : J5604-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MS-VB-29736-BOX-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.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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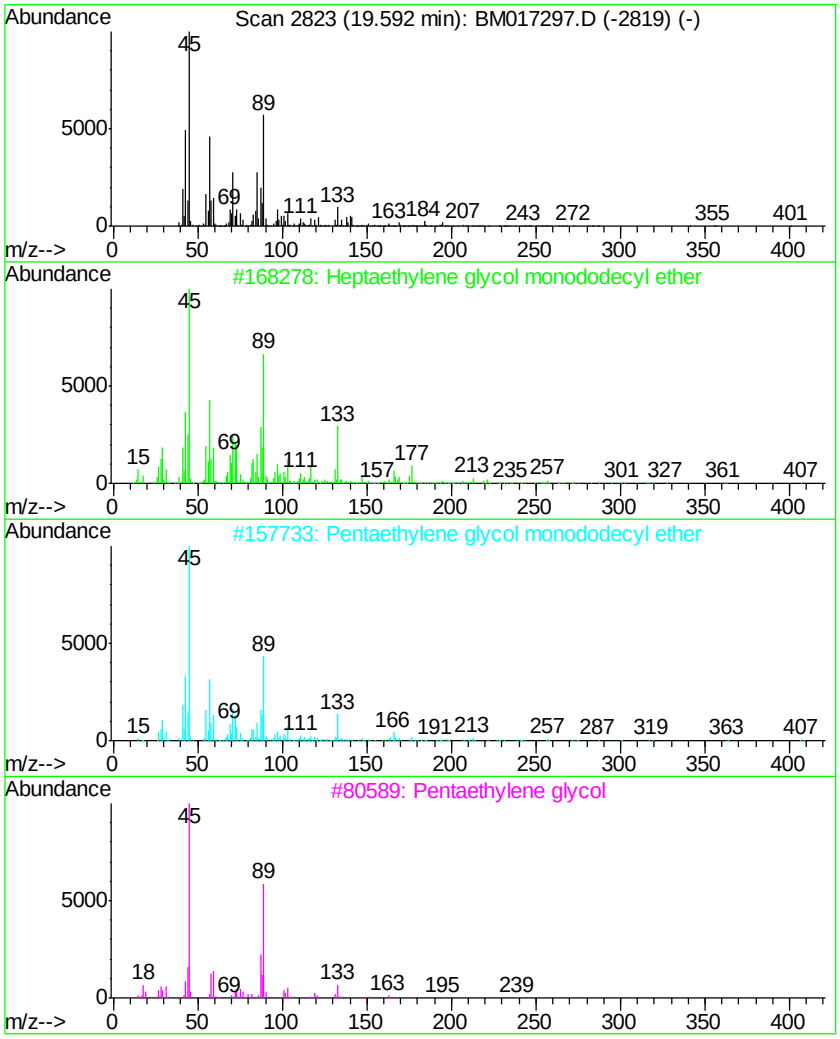
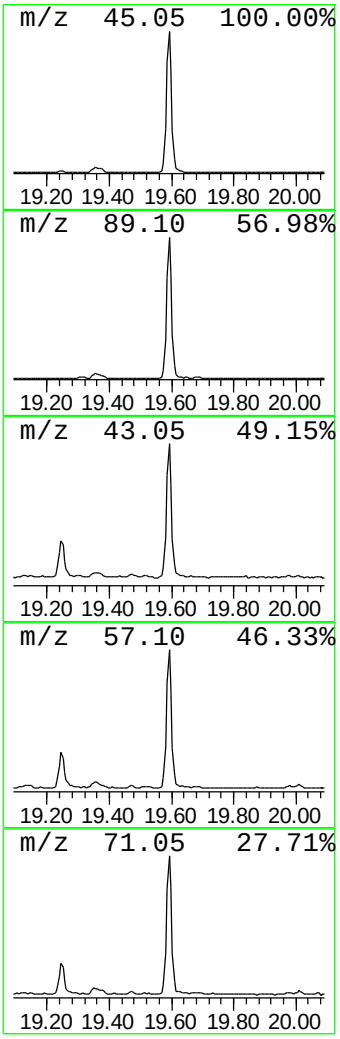
Peak Number 12 Heptaethylene glycol monodo... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.59	21.91 ng	3836610	Chrysene-d12	21.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptaethylene glycol monododecyl...	494	C26H54O8	003055-97-8	72
2	Pentaethylene glycol monododecyl...	406	C22H46O6	003055-95-6	72
3	Pentaethylene glycol	238	C10H22O6	004792-15-8	68
4	Heptaethylene glycol	326	C14H30O8	005617-32-3	64
5	Hexagol	282	C12H26O7	002615-15-8	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM102318\
Data File : BM017297.D
Acq On : 23 Oct 2018 22:42
Operator : MJ/SJ
Sample : J5604-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MS-VB-29736-BOX-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown5.17	5.17	25.8	ng	7645940	1	7.66	5930170	20.0
Phenol, 2-fluoro-	5.40	10.4	ng	3067450	1	7.66	5930170	20.0
Ethanol, 2-butoxy-	5.89	774.1	ng	229530000	1	7.66	5930170	20.0
unknown7.20	7.20	22.5	ng	6666290	1	7.66	5930170	20.0
3-Oxabicyclo[3.3....	11.70	22.6	ng	3083290	2	10.43	2732050	20.0
unknown13.26	13.26	38.0	ng	5907650	3	14.30	3106290	20.0
Tetracyclo[4.2.1....	14.72	19.0	ng	2955700	3	14.30	3106290	20.0
unknown15.85	15.85	36.9	ng	6049120	4	17.05	3281020	20.0
Hexagol	17.91	35.8	ng	5870190	4	17.05	3281020	20.0
n-Hexadecanoic acid	17.96	14.4	ng	2361050	4	17.05	3281020	20.0
Heptaethylene gly...	19.59	21.9	ng	3836610	5	21.24	3501860	20.0