LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM102318\
Data File : BM017298.D
Acq On : 23 Oct 2018 23:18
Operator : MJ/SJ
Sample : J5604-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MS-VB-25868-BOX-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_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	5148214	7095757	3.28%	1.933%
2	5.387	401	408	418	rVB	1456369	2934466	1.35%	0.800%
3	5.887	467	493	496	rBV2	41233327	216649589	100.00%	59.033%
4	6.846	649	656	669	rVB2	1256843	2497963	1.15%	0.681%
5	7.204	709	717	727	rBV	3902842	6175591	2.85%	1.683%
6	7.975	842	848	855	rBV	3756356	5906186	2.73%	1.609%
7	8.816	951	991	996	rBV2	8421283	46892084	21.64%	12.777%
8	10.434	1257	1266	1276	rBV	1369036	2478892	1.14%	0.675%
9	11.698	1472	1481	1489	rVV4	1066613	3119153	1.44%	0.850%
10	12.916	1681	1688	1694	rBV	6506561	9547218	4.41%	2.601%
11	13.263	1742	1747	1760	rVB2	4304609	6270679	2.89%	1.709%
12	14.298	1913	1923	1930	rBV2	1758089	2922705	1.35%	0.796%
13	14.721	1989	1995	2003	rVB2	1745788	2980376	1.38%	0.812%
14	15.798	2171	2178	2183	rBV	4849356	7051400	3.25%	1.921%
15	15.851	2183	2187	2194	rVV	4302630	5886494	2.72%	1.604%
16	16.574	2305	2310	2318	rBV	1590293	2275282	1.05%	0.620%
17	17.051	2386	2391	2398	rVB2	2034120	2951260	1.36%	0.804%
18	17.910	2532	2537	2542	rVV	4308903	5512296	2.54%	1.502%
19	17.962	2542	2546	2552	rVB	2848709	3432044	1.58%	0.935%
20	19.592	2819	2823	2829	rVB	3485741	3954856	1.83%	1.078%
21	19.692	2835	2840	2845	rVB	8602788	10808159	4.99%	2.945%
22	20.945	3049	3053	3055	rBV	1964554	2351737	1.09%	0.641%
23	21.245	3100	3104	3114	rVB	2719279	3555918	1.64%	0.969%
24	23.456	3474	3480	3494	rVB	2042941	3745359	1.73%	1.021%

Sum of corrected areas: 366995464

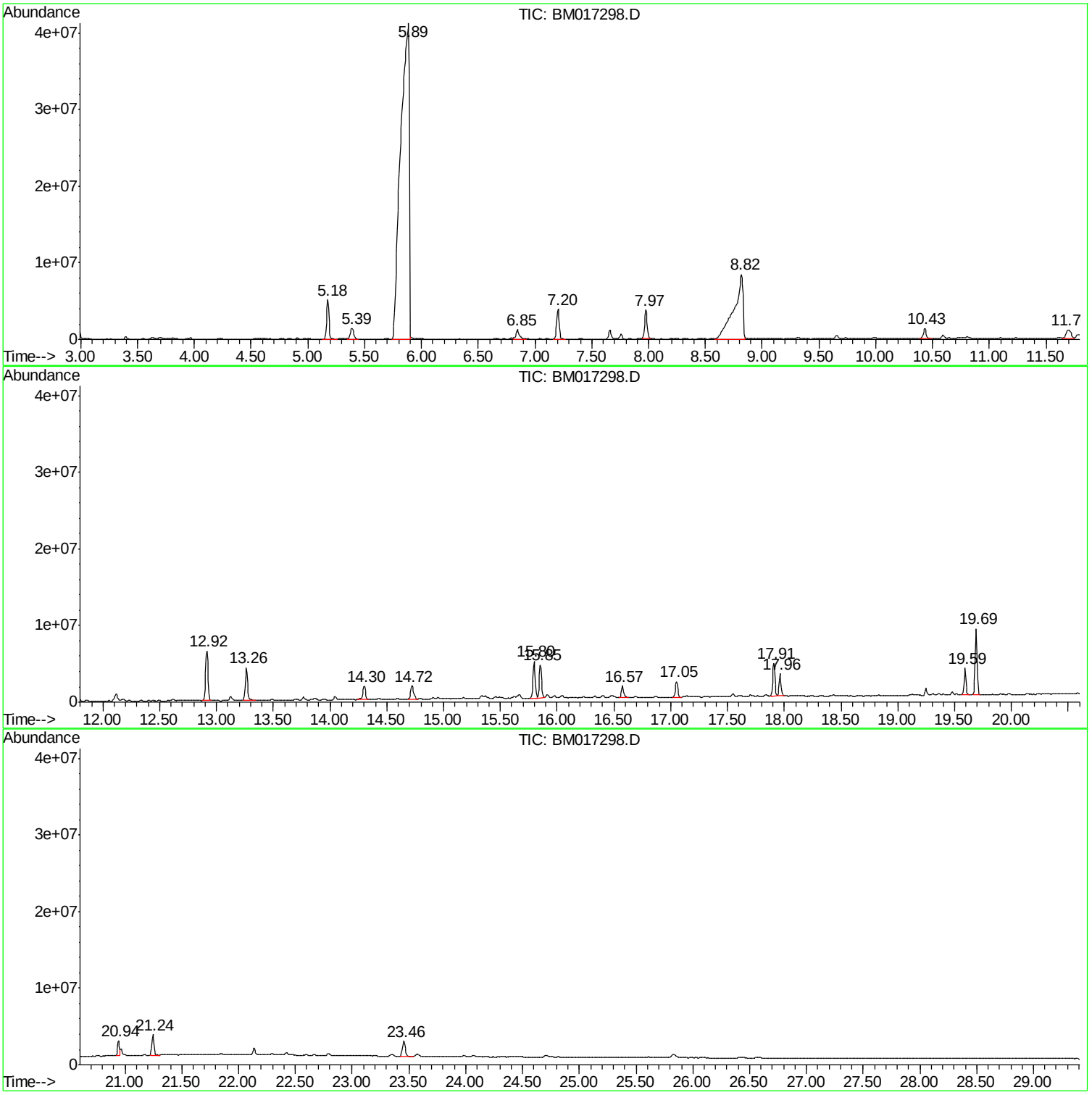
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM102318\
Data File : BM017298.D
Acq On : 23 Oct 2018 23:18
Operator : MJ/SJ
Sample : J5604-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-VB-25868-BOX-1

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM102318\
Data File : BM017298.D
Acq On : 23 Oct 2018 23:18
Operator : MJ/SJ
Sample : J5604-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MS-VB-25868-BOX-1

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

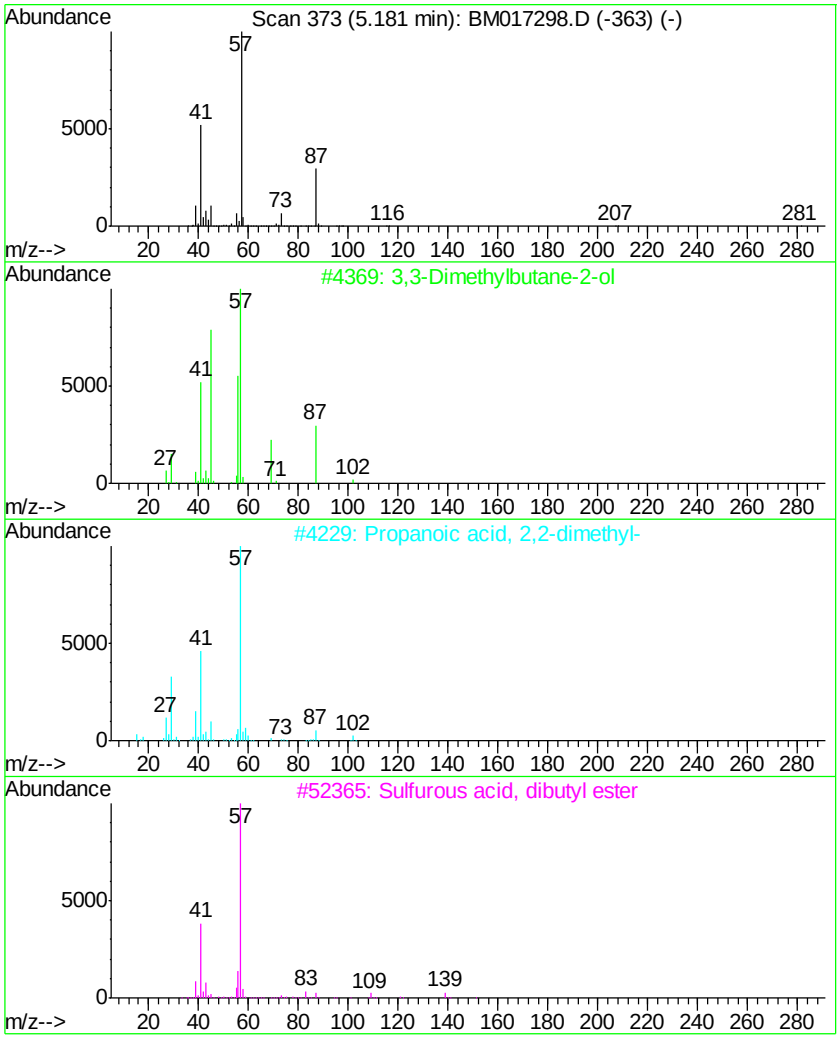
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

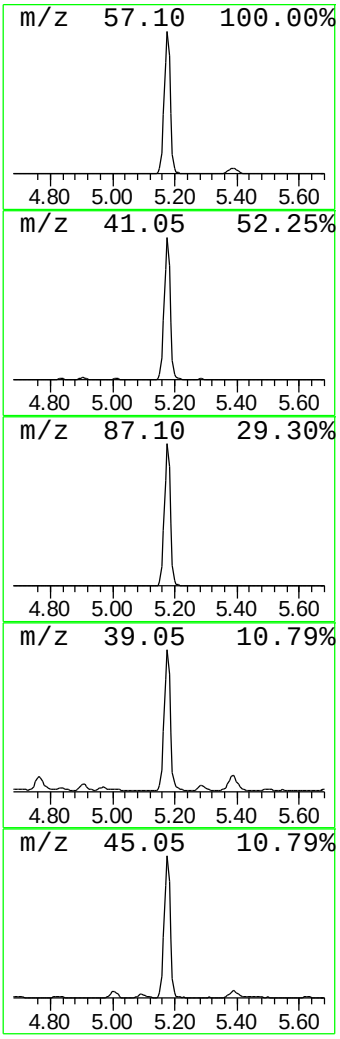
****

Peak Number 1 unknown5.18 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	24.03 ng	7095760	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	Sulfurous acid, dibutyl ester	194	C8H18O3S	000626-85-7	25
4	1-Propanol, 2,2-dimethyl-	88	C5H12O	000075-84-3	25
5	Propanedioic acid, oxo-, bis(2-m...	230	C11H18O5	092778-43-3	23





Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM102318\
Data File : BM017298.D
Acq On : 23 Oct 2018 23:18
Operator : MJ/SJ
Sample : J5604-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MS-VB-25868-BOX-1

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

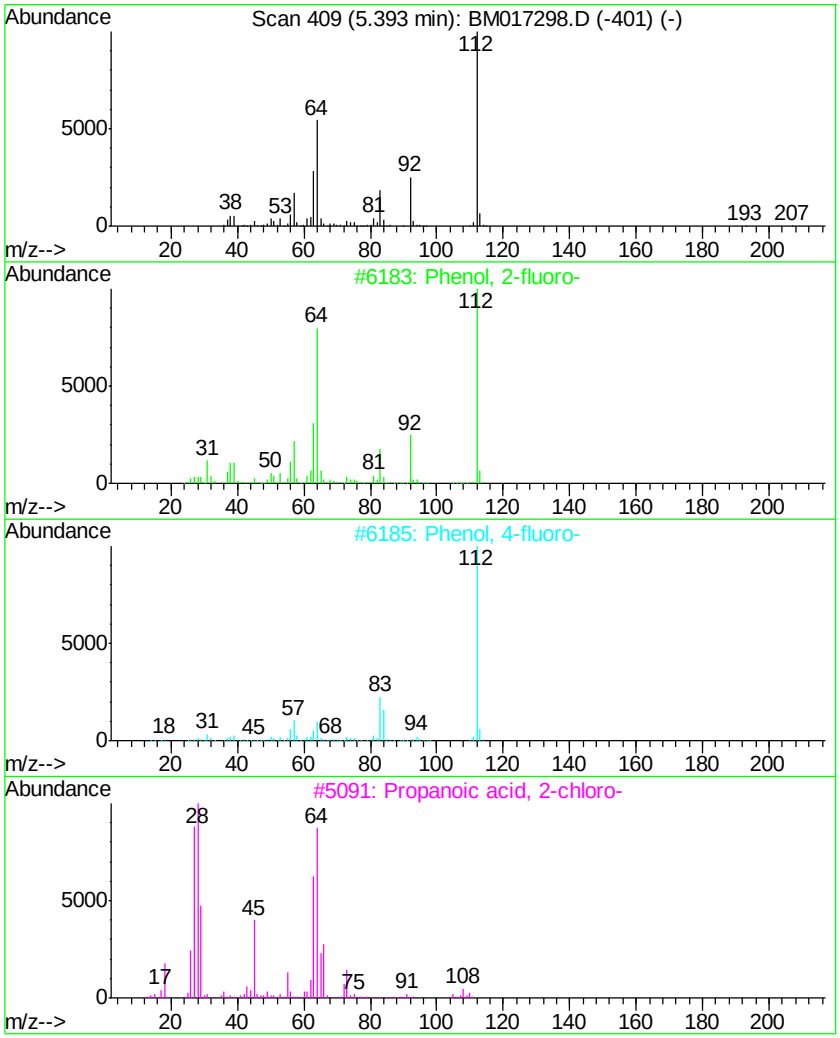
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

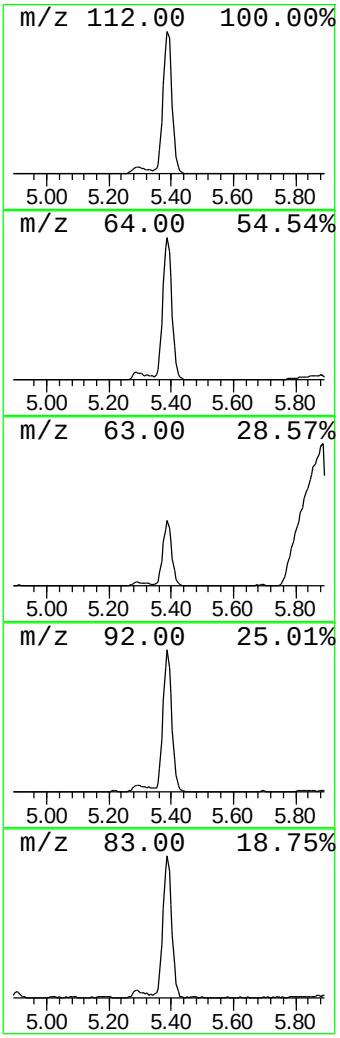
****

Peak Number 2 Phenol, 2-fluoro- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.39	9.94 ng	2934470	1,4-Dichlorobenzene-d4	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-fluoro-	112	C6H5FO	000367-12-4	91
2	Phenol, 4-fluoro-	112	C6H5FO	000371-41-5	30
3	Propanoic acid, 2-chloro-	108	C3H5ClO2	000598-78-7	23
4	Cysteic acid	169	C3H7NO5S	1000131-23-1	17
5	Phenol, 3-fluoro-	112	C6H5FO	000372-20-3	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM102318\
Data File : BM017298.D
Acq On : 23 Oct 2018 23:18
Operator : MJ/SJ
Sample : J5604-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MS-VB-25868-BOX-1

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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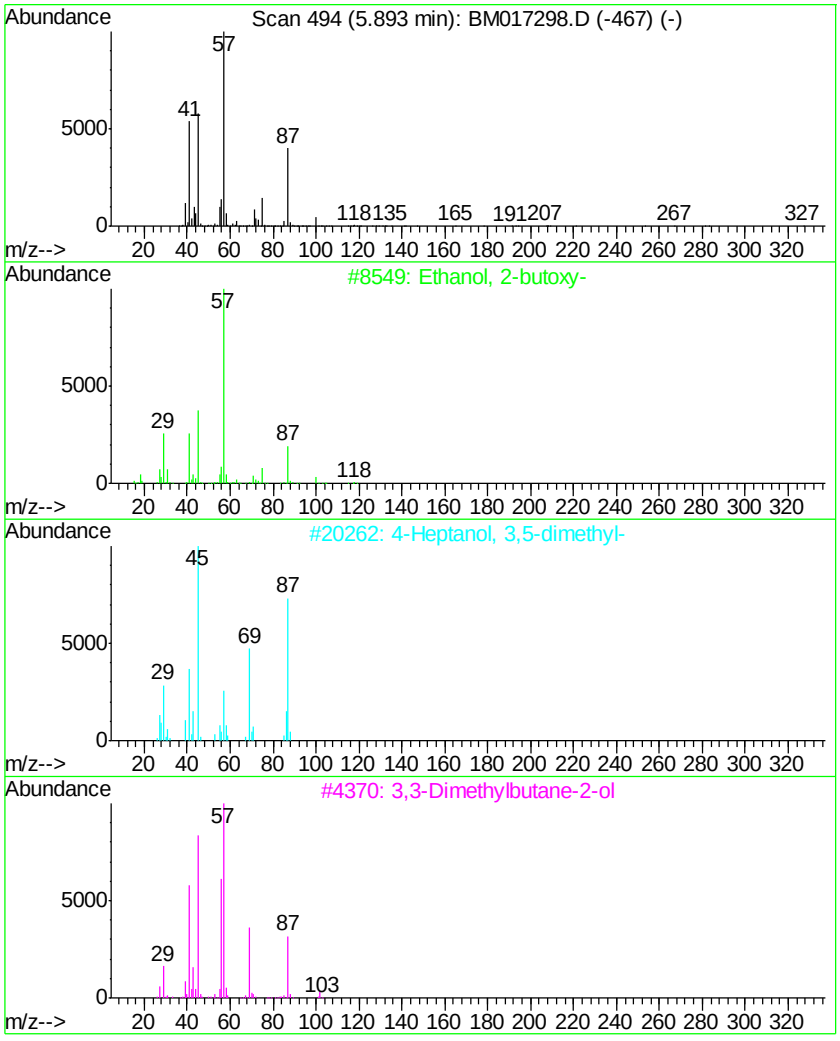
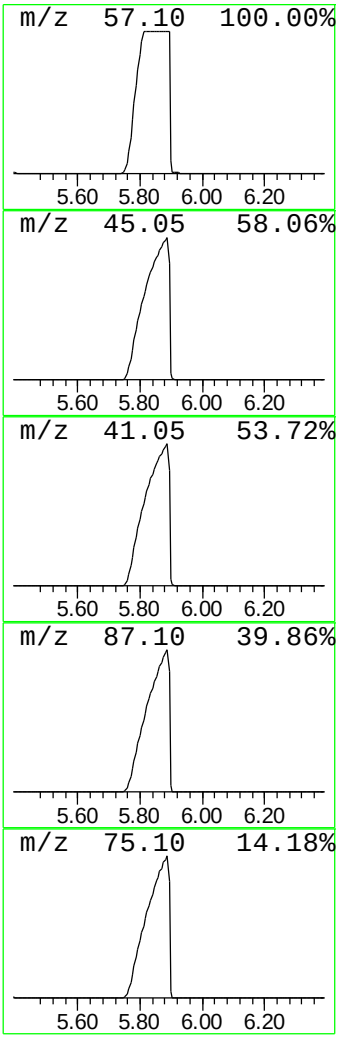
Peak Number 3 Ethanol, 2-butoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.89	733.64 ng	216650000	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	38
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	38
5	4,5-Octanediol, 3,6-dimethyl-	174	C10H22O2	1000153-21-1	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM102318\
Data File : BM017298.D
Acq On : 23 Oct 2018 23:18
Operator : MJ/SJ
Sample : J5604-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MS-VB-25868-BOX-1

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

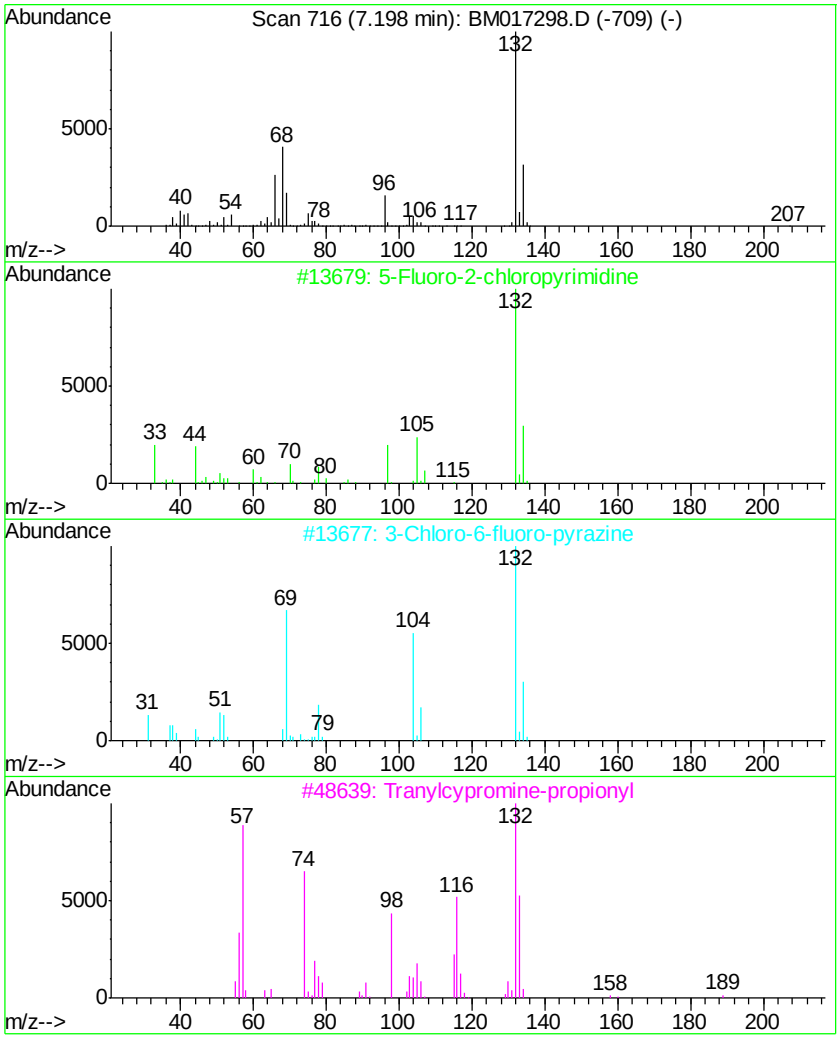
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

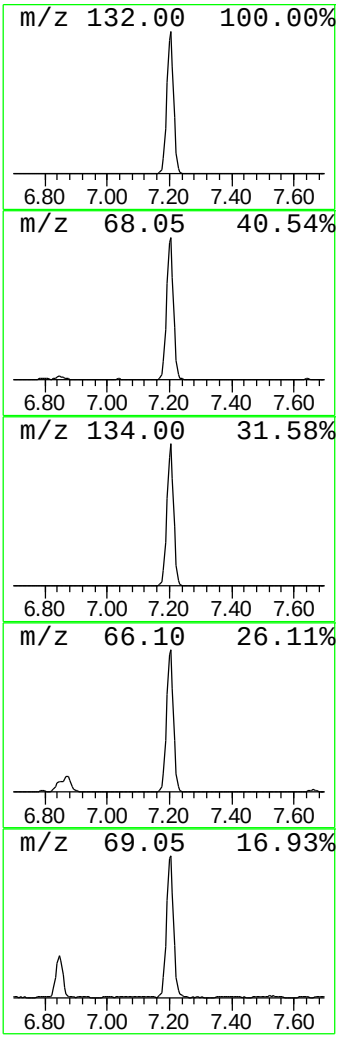
****

Peak Number 4 unknown7.20 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	20.91 ng	6175590	1,4-Dichlorobenzene-d4	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
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	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM102318\
Data File : BM017298.D
Acq On : 23 Oct 2018 23:18
Operator : MJ/SJ
Sample : J5604-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MS-VB-25868-BOX-1

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

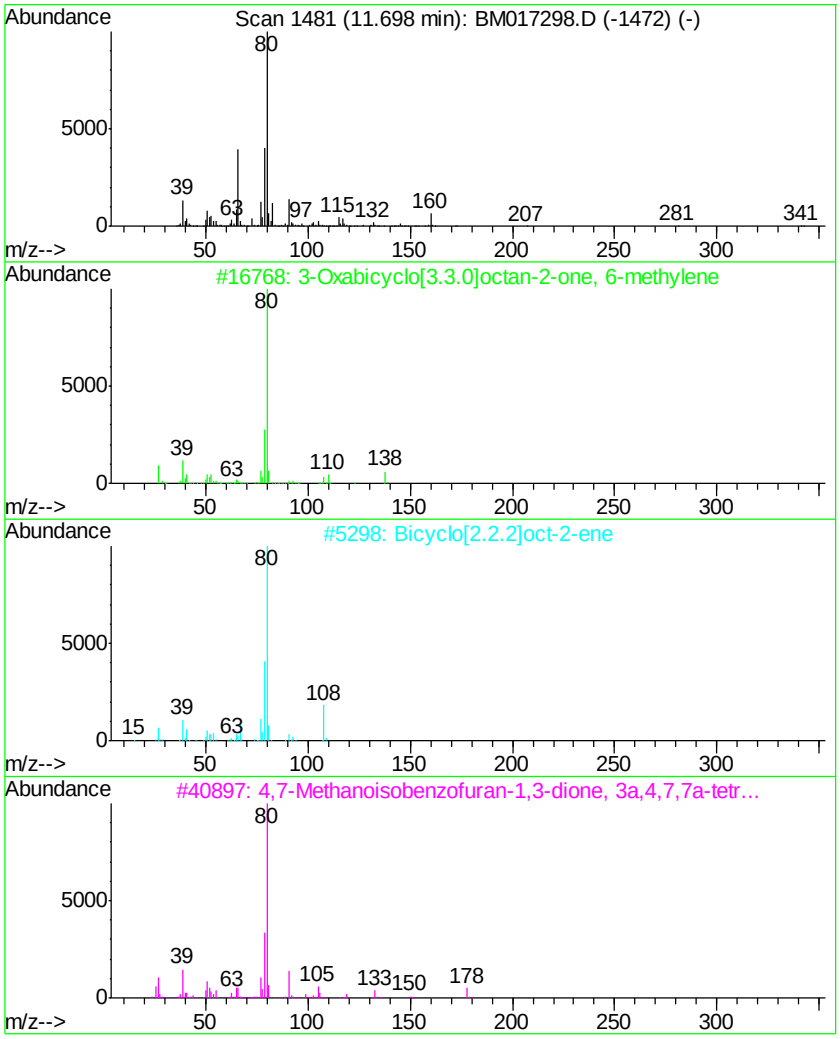
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

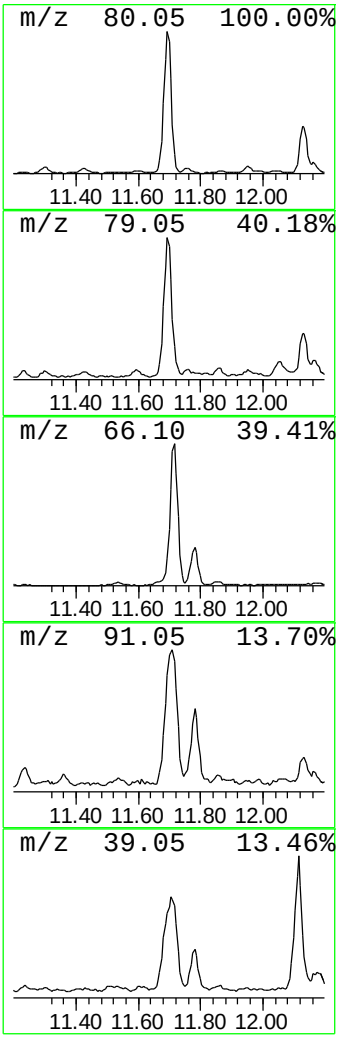
****

Peak Number 6 3-Oxabicyclo[3.3.0]octan-2-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	25.17 ng	3119150	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	50
2	Bicyclo[2.2.2]oct-2-ene	108	C8H12	000931-64-6	50
3	4,7-Methanoisobenzofuran-1,3-dio...	178	C10H10O3	000117-40-8	50
4	Bicyclo[3.2.0]hept-2-ene, 2-methyl-	108	C8H12	094122-58-4	50
5	Bicyclo[2.2.1]hept-2-ene, 2-methyl-	108	C8H12	000694-92-8	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM102318\
Data File : BM017298.D
Acq On : 23 Oct 2018 23:18
Operator : MJ/SJ
Sample : J5604-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MS-VB-25868-BOX-1

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

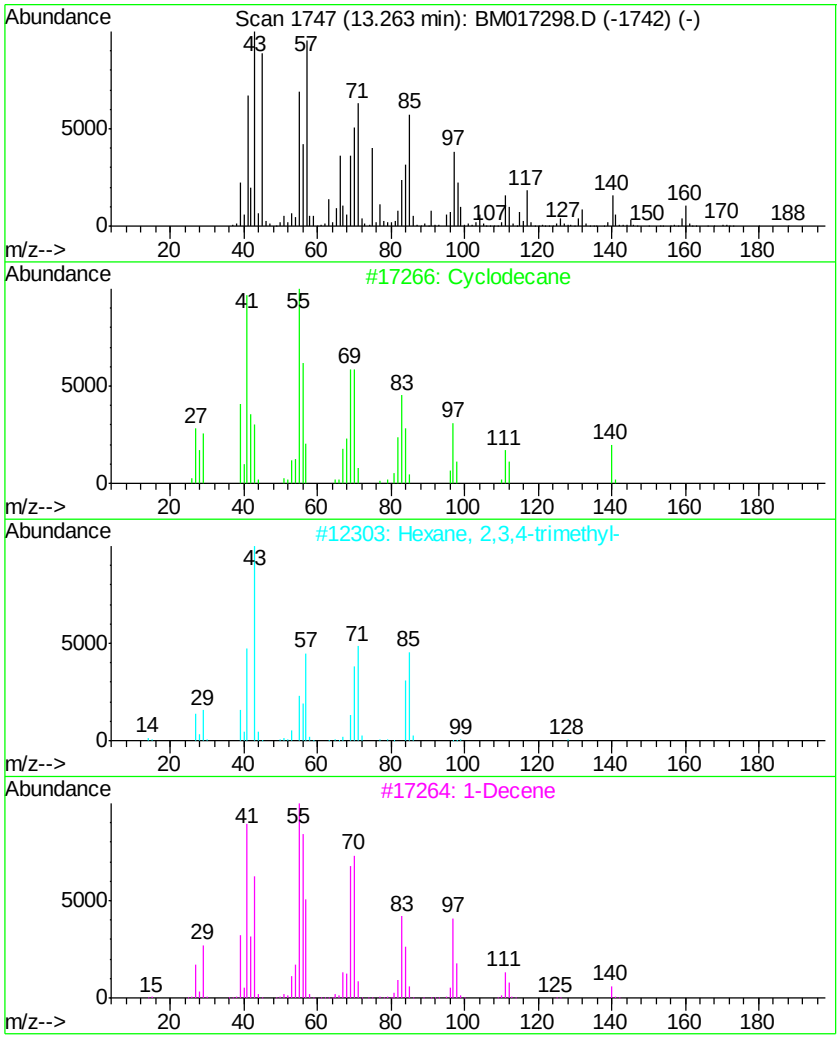
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

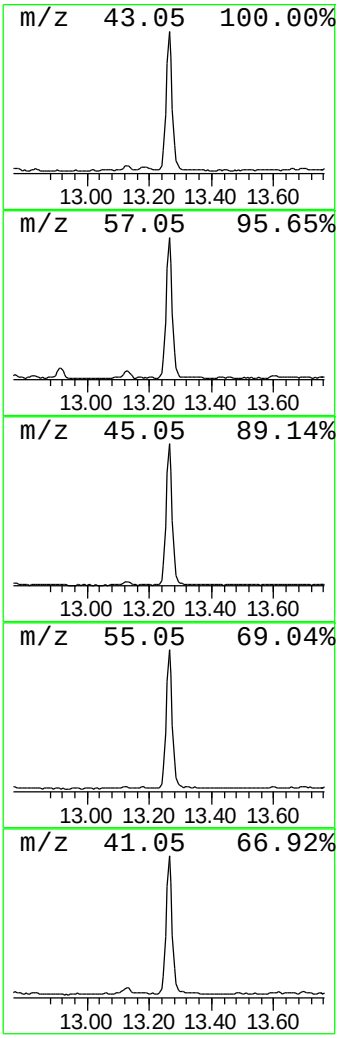
****

Peak Number 7 unknown13.26 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.26	42.91 ng	6270680	Acenaphthene-d10	14.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclodecane	140	C10H20	000293-96-9	38
2	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	38
3	1-Decene	140	C10H20	000872-05-9	35
4	Hexane, 1-(hexyloxy)-3-methyl-	200	C13H28O	074421-18-4	22
5	5-Undecene, 8-methyl-, (E)-	168	C12H24	039546-85-5	22





Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM102318\
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Acq On : 23 Oct 2018 23:18
Operator : MJ/SJ
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Misc :
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Instrument : BNA_M
ClientSampleId : MS-VB-25868-BOX-1

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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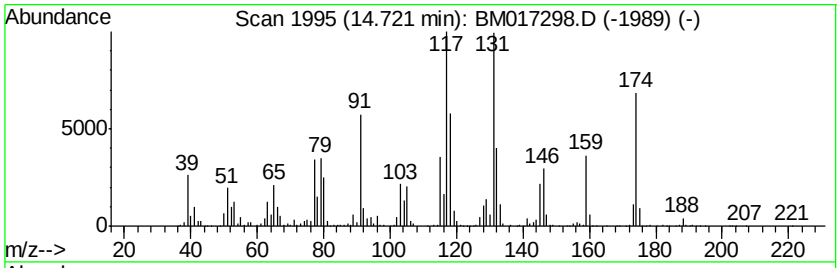
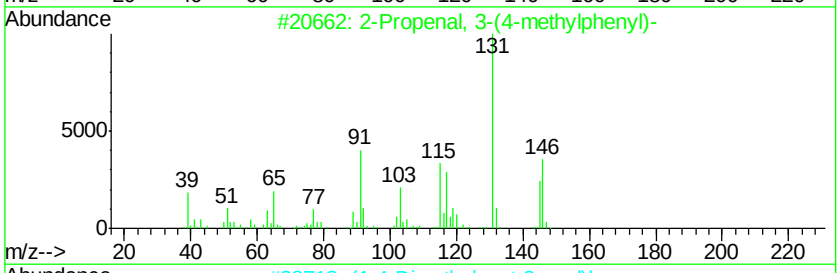
****

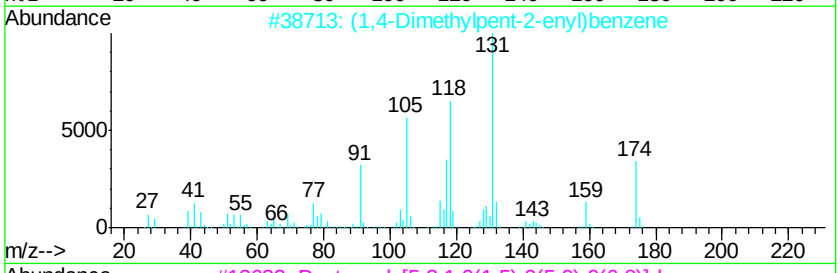
Peak Number 8 unknown14.72 Concentration Rank 10

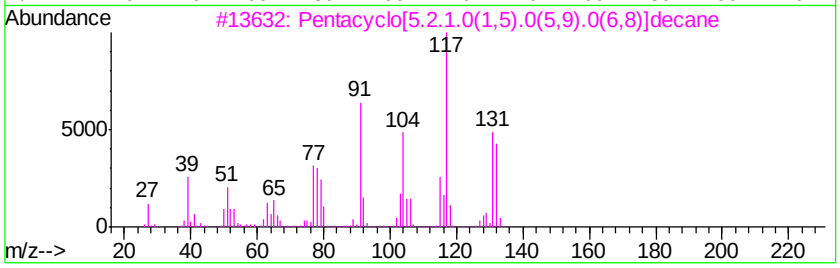
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	20.39 ng	2980380	Acenaphthene-d10	14.30

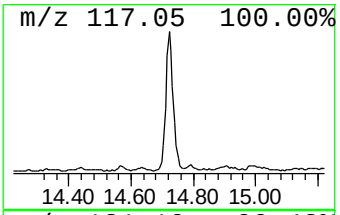
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenal, 3-(4-methylphenyl)-	146	C10H10O	001504-75-2	46
2	(1,4-Dimethylpent-2-enyl)benzene	174	C13H18	1000184-97-9	45
3	Pentacyclo[5.2.1.0(1,5).0(5,9).0...	132	C10H12	1000185-59-0	45
4	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	42
5	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	38

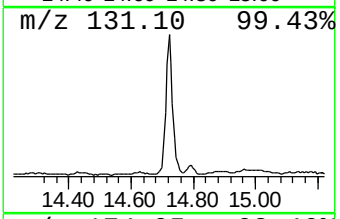


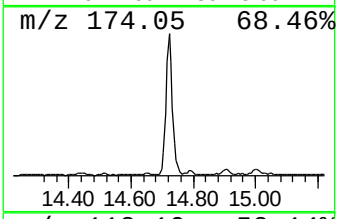


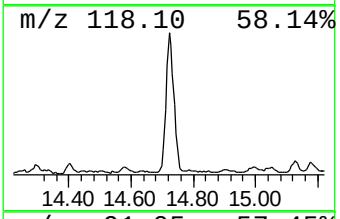


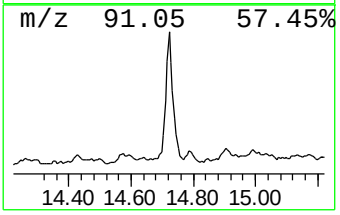












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ClientSampleId : MS-VB-25868-BOX-1

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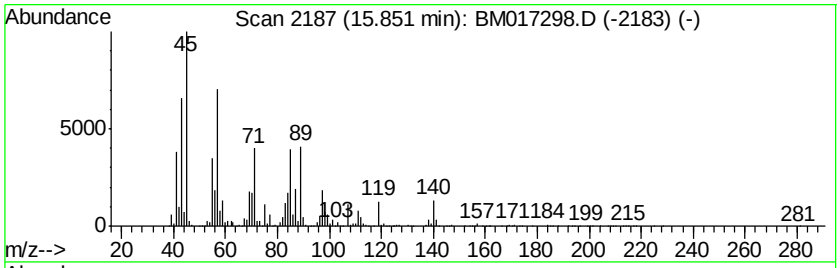
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

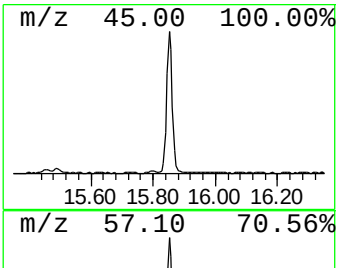
****

Peak Number 9 Propanoic acid, 2-methyl-, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.85	39.89 ng	5886490	Phenanthrene-d10	17.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, decyl...	228	C14H28O2	005454-22-8	55
2	Methoxyacetic acid, tridecyl ester	272	C16H32O3	1000281-82-0	47
3	Hydroxylamine, O-decyl-	173	C10H23NO	029812-79-1	35
4	Decane, 1,1'-oxybis-	298	C20H42O	002456-28-2	30
5	Decane, 2,4,6-trimethyl-	184	C13H28	062108-27-4	22





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Data File : BM017298.D
Acq On : 23 Oct 2018 23:18
Operator : MJ/SJ
Sample : J5604-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MS-VB-25868-BOX-1

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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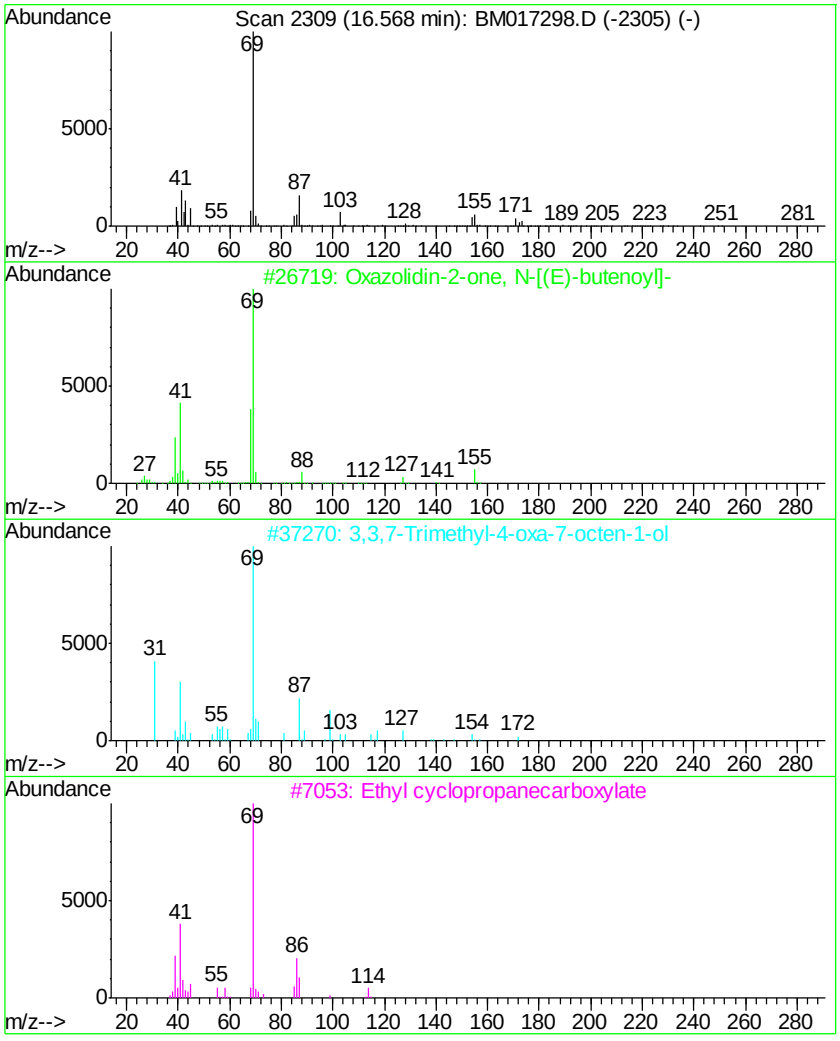
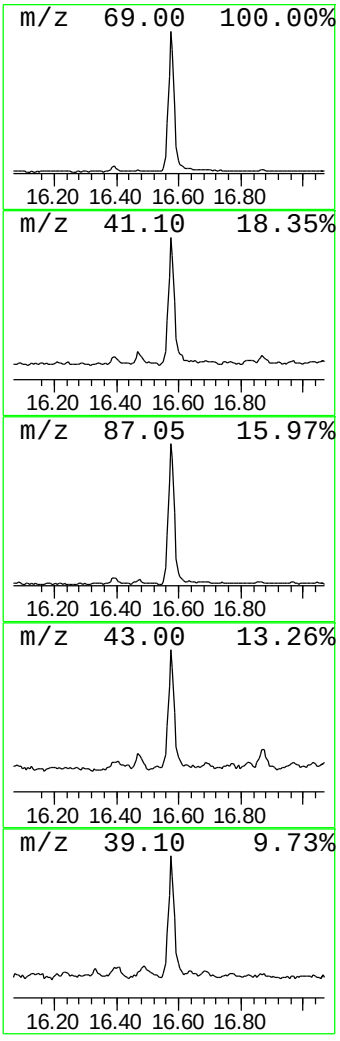
Peak Number 10 unknown16.57 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.57	15.42 ng	2275280	Phenanthrene-d10	17.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxazolidin-2-one, N-[(E)-butenoyl]-	155	C7H9NO3	1000156-45-5	40
2	3,3,7-Trimethyl-4-oxa-7-octen-1-ol	172	C10H20O2	069161-47-3	39
3	Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	38
4	3-Hexanol, 2,5-dimethyl-	130	C8H18O	019550-07-3	9
5	Cyclopropanecarboxylic acid,buty...	142	C8H14O2	054947-39-6	9





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Data File : BM017298.D
Acq On : 23 Oct 2018 23:18
Operator : MJ/SJ
Sample : J5604-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MS-VB-25868-BOX-1

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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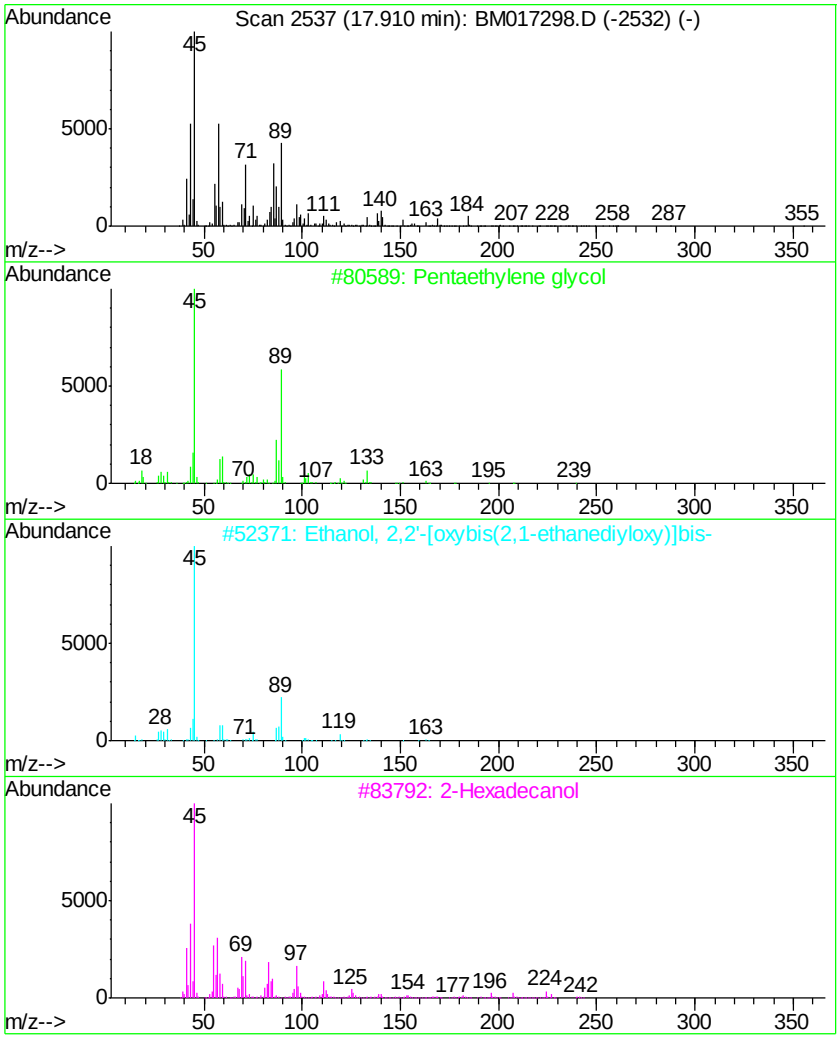
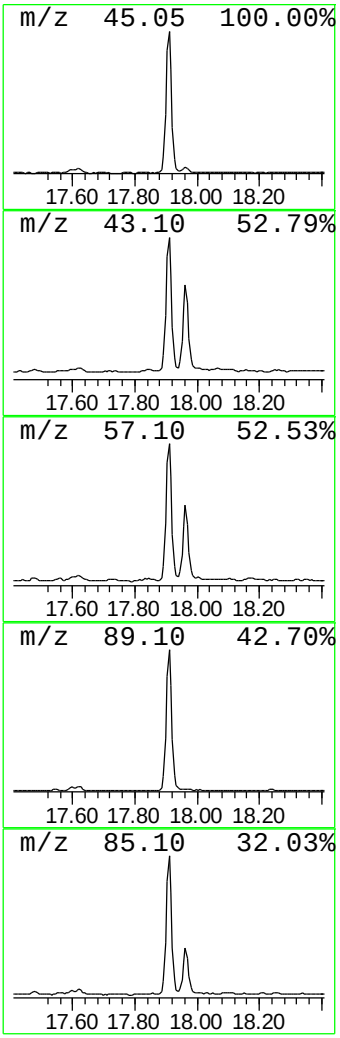
Peak Number 11 Pentaethylene glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.91	37.36 ng	5512300	Phenanthrene-d10	17.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentaethylene glycol	238	C10H22O6	004792-15-8	62
2	Ethanol, 2,2'-[oxybis(2,1-ethane...	194	C8H18O5	000112-60-7	52
3	2-Hexadecanol	242	C16H34O	014852-31-4	50
4	Diisopropyl ether	102	C6H14O	000108-20-3	38
5	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	38





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Data File : BM017298.D
Acq On : 23 Oct 2018 23:18
Operator : MJ/SJ
Sample : J5604-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MS-VB-25868-BOX-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
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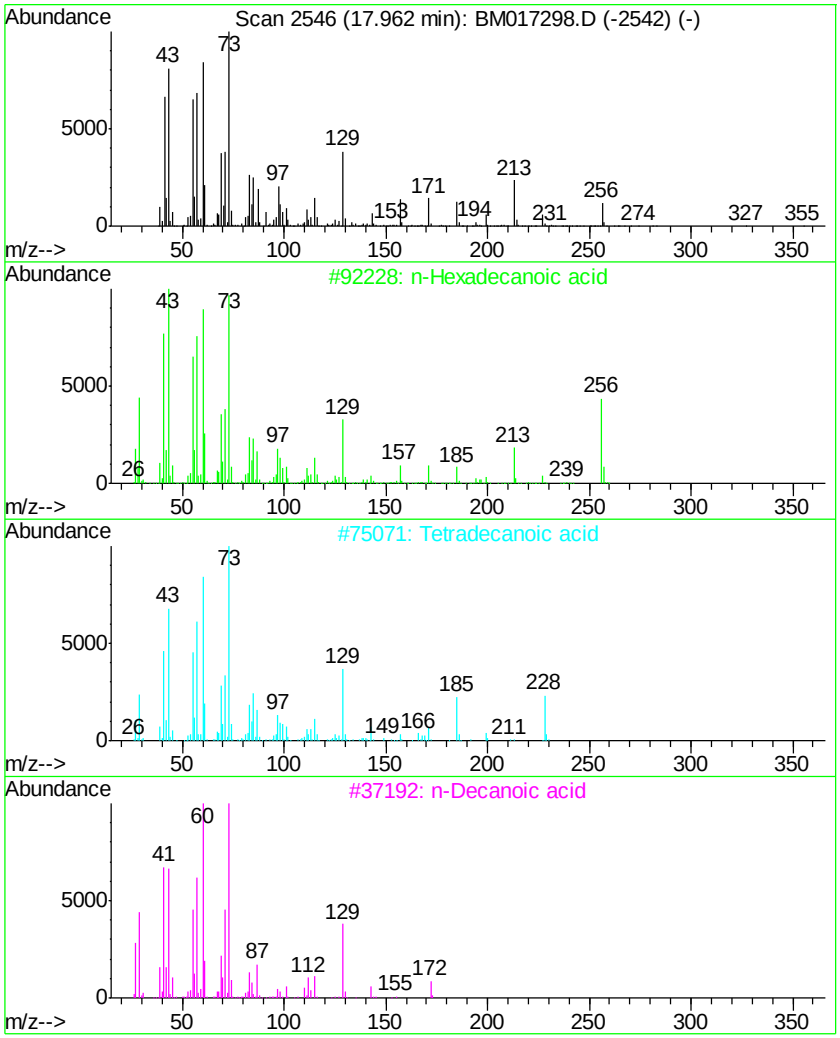
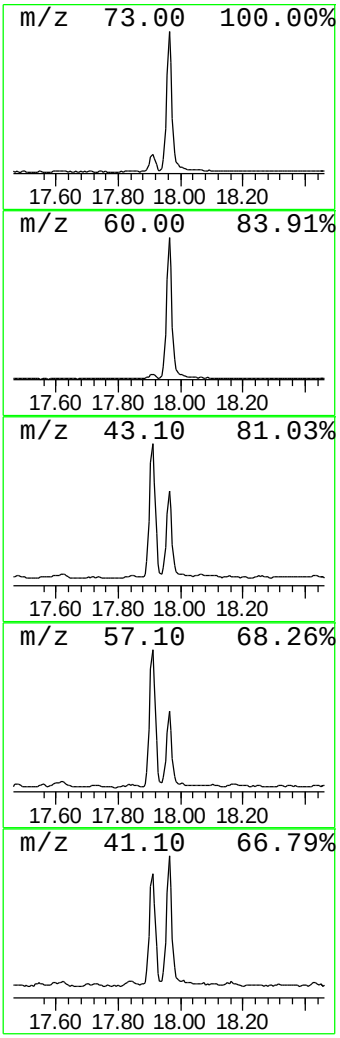
Peak Number 12 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.96	23.26 ng	3432040	Phenanthrene-d10	17.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3	n-Decanoic acid	172	C10H20O2	000334-48-5	76
4	Tridecanoic acid	214	C13H26O2	000638-53-9	60
5	Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	25





Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM102318\
Data File : BM017298.D
Acq On : 23 Oct 2018 23:18
Operator : MJ/SJ
Sample : J5604-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MS-VB-25868-BOX-1

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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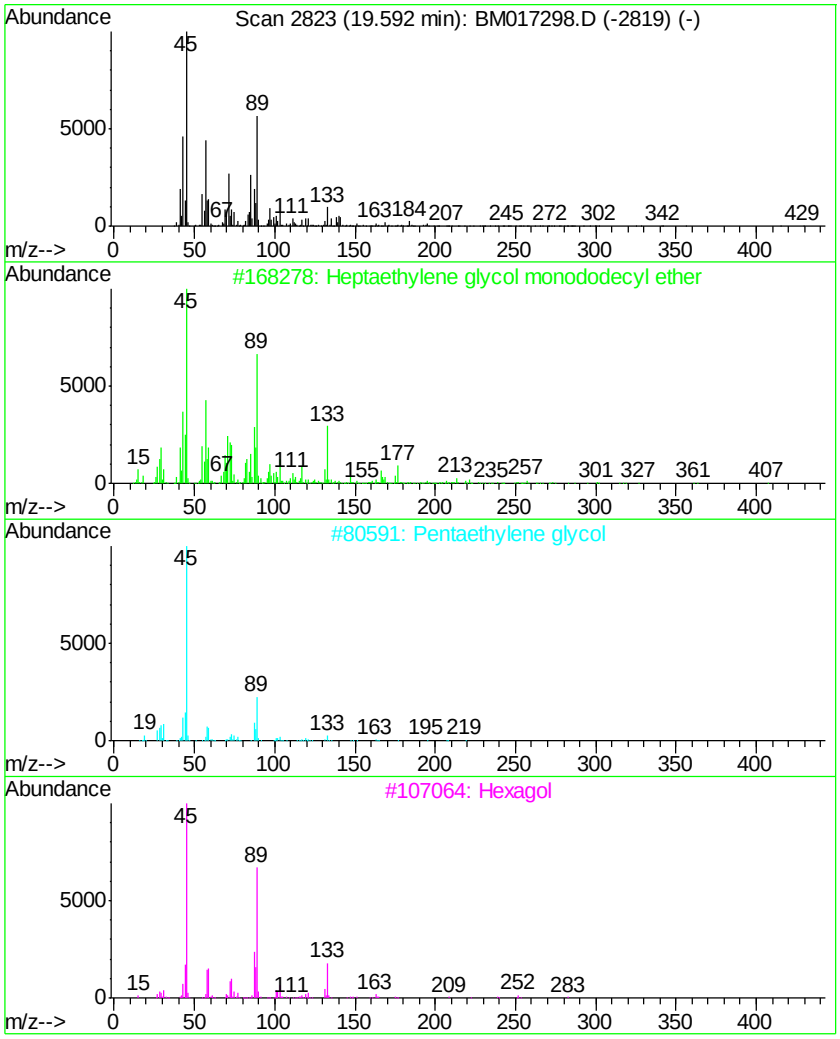
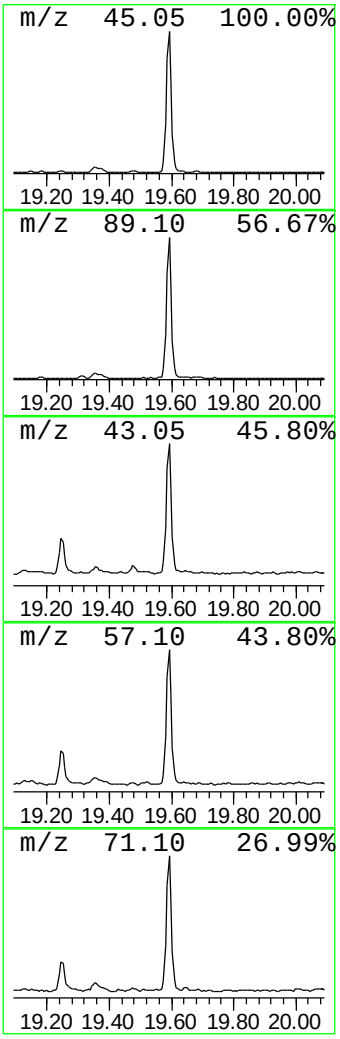
Peak Number 13 Heptaethylene glycol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.59	22.24 ng	3954860	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	238	C10H22O6	004792-15-8	68
3	Hexagol	282	C12H26O7	002615-15-8	64
4	Heptaethylene glycol	326	C14H30O8	005617-32-3	64
5	1,4,7,10,13,16-Hexaoxanonadecane...	320	C16H32O6	1000163-65-3	53





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Data File : BM017298.D
Acq On : 23 Oct 2018 23:18
Operator : MJ/SJ
Sample : J5604-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MS-VB-25868-BOX-1

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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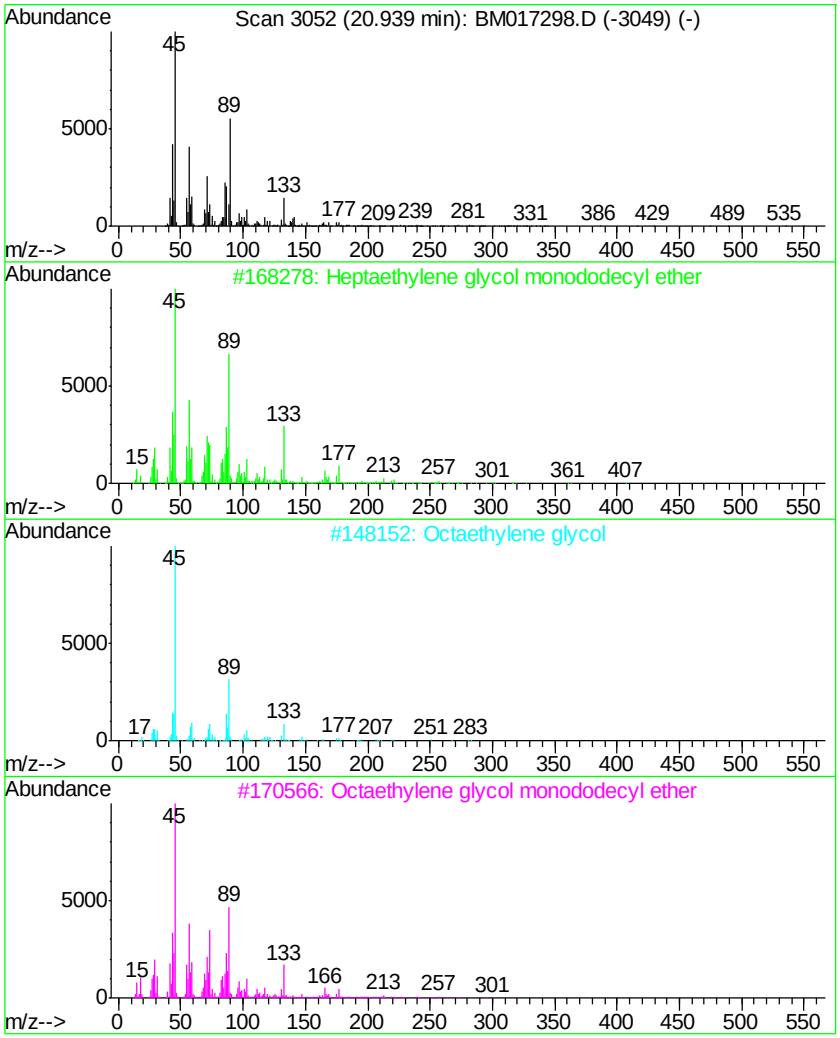
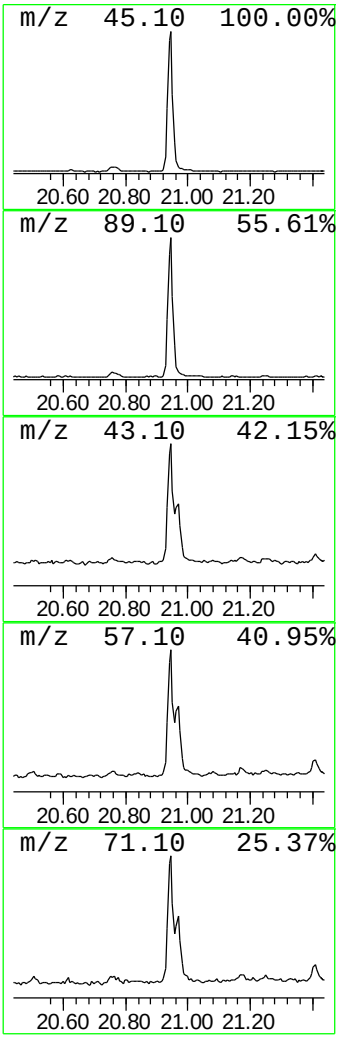
Peak Number 14 Heptaethylene glycol monodo... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.94	13.23 ng	2351740	Chrysene-d12	21.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptaethylene glycol monododecyl...	494	C26H54O8	003055-97-8	78
2	Octaethylene glycol	370	C16H34O9	1000289-34-2	74
3	Octaethylene glycol monododecyl ...	538	C28H58O9	003055-98-9	72
4	Heptaethylene glycol	326	C14H30O8	005617-32-3	72
5	Pentaethylene glycol monododecyl...	406	C22H46O6	003055-95-6	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM102318\
Data File : BM017298.D
Acq On : 23 Oct 2018 23:18
Operator : MJ/SJ
Sample : J5604-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MS-VB-25868-BOX-1

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
unknown5.18	5.18	24.0	ng	7095760	1	7.66	5906190	20.0
Phenol, 2-fluoro-	5.39	9.9	ng	2934470	1	7.66	5906190	20.0
Ethanol, 2-butoxy-	5.89	733.6	ng	216650000	1	7.66	5906190	20.0
unknown7.20	7.20	20.9	ng	6175590	1	7.66	5906190	20.0
3-Oxabicyclo[3.3....	11.70	25.2	ng	3119150	2	10.43	2478890	20.0
unknown13.26	13.26	42.9	ng	6270680	3	14.30	2922710	20.0
unknown14.72	14.72	20.4	ng	2980380	3	14.30	2922710	20.0
Propanoic acid, 2...	15.85	39.9	ng	5886490	4	17.05	2951260	20.0
unknown16.57	16.57	15.4	ng	2275280	4	17.05	2951260	20.0
Pentaethylene glycol	17.91	37.4	ng	5512300	4	17.05	2951260	20.0
n-Hexadecanoic acid	17.96	23.3	ng	3432040	4	17.05	2951260	20.0
Heptaethylene glycol	19.59	22.2	ng	3954860	5	21.24	3555920	20.0
Heptaethylene gly...	20.94	13.2	ng	2351740	5	21.24	3555920	20.0