LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021219\
Data File : BM018783.D
Acq On : 12 Feb 2019 21:29
Operator : JU/SJ
Sample : K1460-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-2-20190208

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-BM021119.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	4.628	251	262	267	rBV	195218	408461	1.49%	0.301%
2	5.304	370	377	388	rBV	4100591	5821659	21.27%	4.285%
3	6.745	614	622	628	rBV	147191	283559	1.04%	0.209%
4	6.887	638	646	657	rBV	2544869	4558609	16.65%	3.355%
5	7.251	700	708	721	rBV	6777686	10926404	39.92%	8.041%
6	7.710	780	786	801	rBV	1423552	2342083	8.56%	1.724%
7	8.028	832	840	851	rBV	5516920	8838586	32.29%	6.505%
8	8.881	978	985	993	rBV	4527302	7648581	27.94%	5.629%
9	9.922	1155	1162	1168	rVB	253154	418254	1.53%	0.308%
10	10.275	1213	1222	1233	rBV	198925	395191	1.44%	0.291%
11	10.504	1254	1261	1267	rBV	1901938	3168740	11.58%	2.332%
12	12.327	1565	1571	1578	rBV	186430	342736	1.25%	0.252%
13	12.980	1674	1682	1697	rBV	11689345	17262433	63.06%	12.705%
14	14.363	1907	1917	1923	rBV2	2757939	4246067	15.51%	3.125%
15	14.445	1923	1931	1954	rVV	4430938	8773323	32.05%	6.457%
16	15.862	2165	2172	2186	rBV	10324065	14476993	52.89%	10.655%
17	17.115	2379	2385	2396	rBV	3676006	5214539	19.05%	3.838%
18	17.304	2412	2417	2425	rBV	374175	580724	2.12%	0.427%
19	19.750	2827	2833	2844	rBV	22357004	27374003	100.00%	20.146%
20	21.303	3093	3097	3103	rBV	5008734	6387759	23.34%	4.701%
21	22.339	3270	3273	3282	rVB2	243489	342419	1.25%	0.252%
22	23.568	3475	3482	3495	rVB	3228138	6064798	22.16%	4.463%

Sum of corrected areas: 135875921

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021219\
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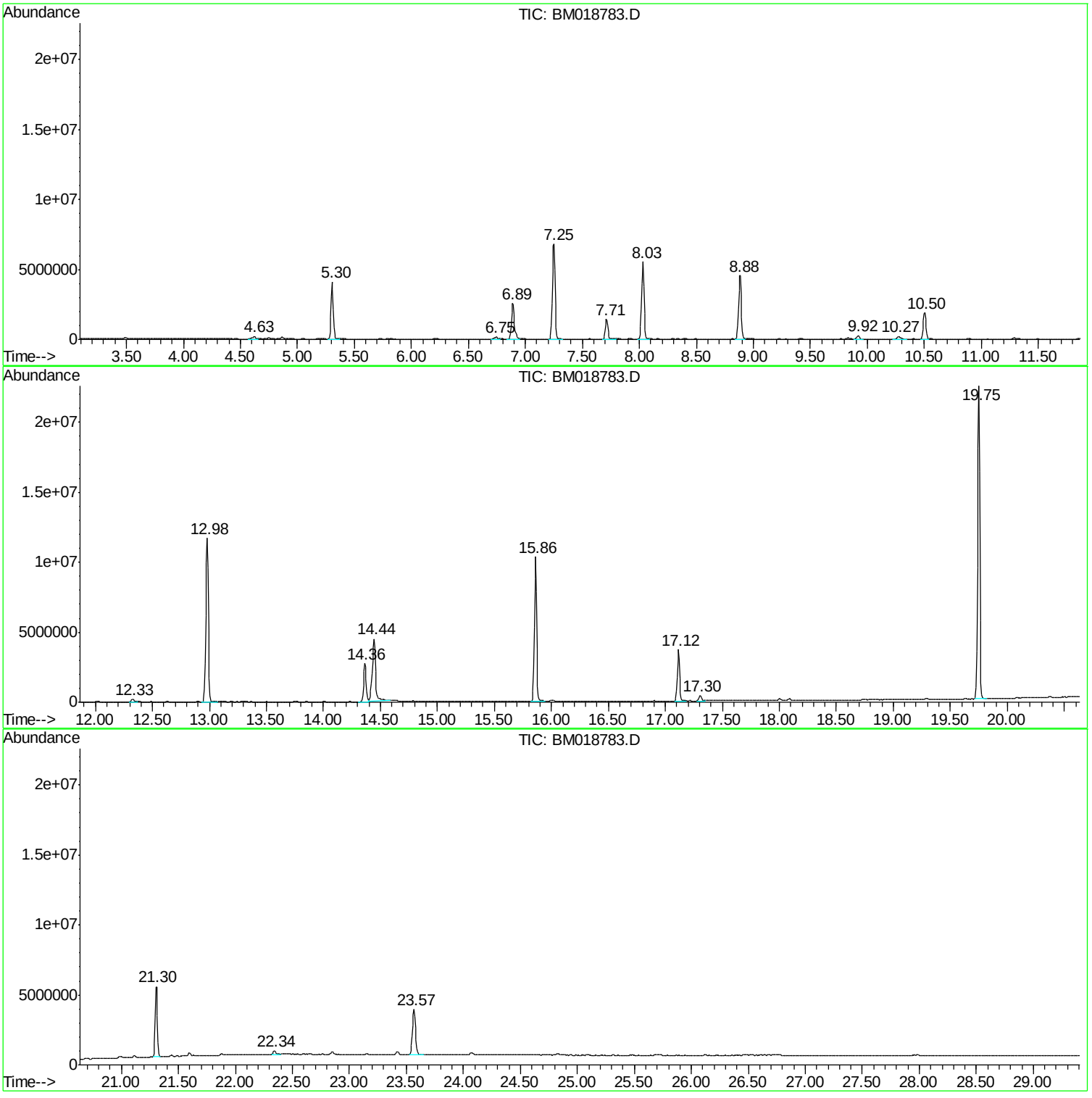
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-2-20190208

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.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\BM021219\
Data File : BM018783.D
Acq On : 12 Feb 2019 21:29
Operator : JU/SJ
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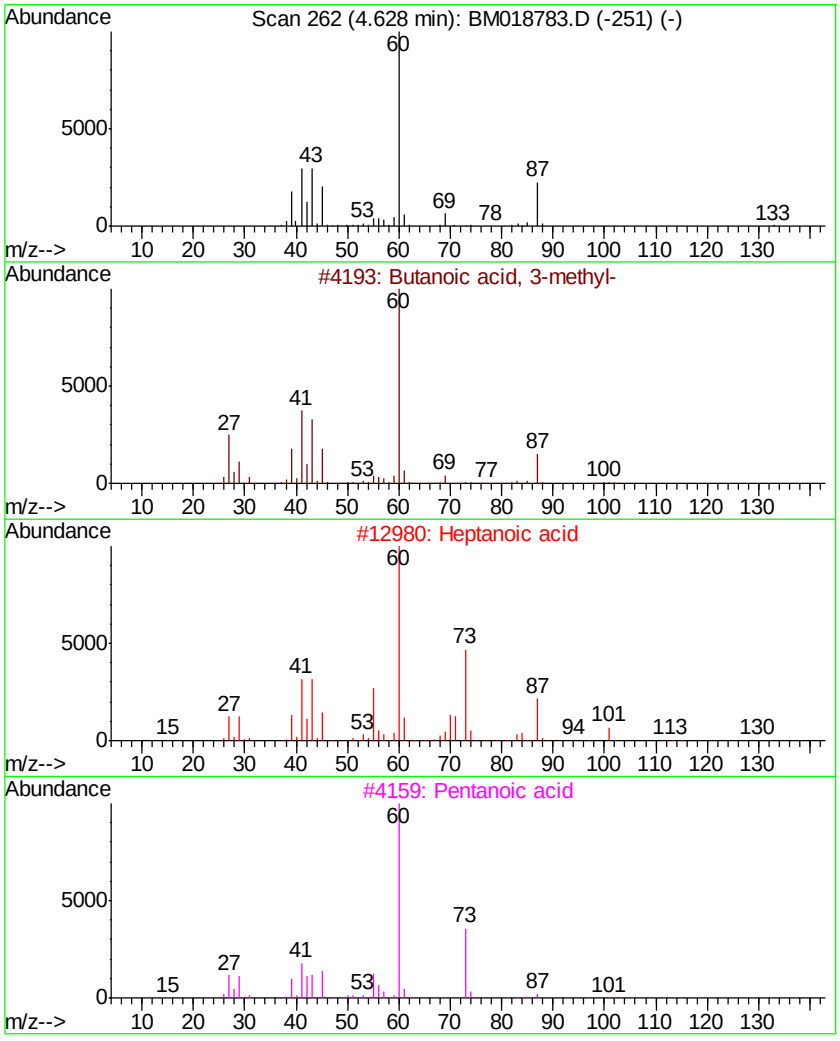
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

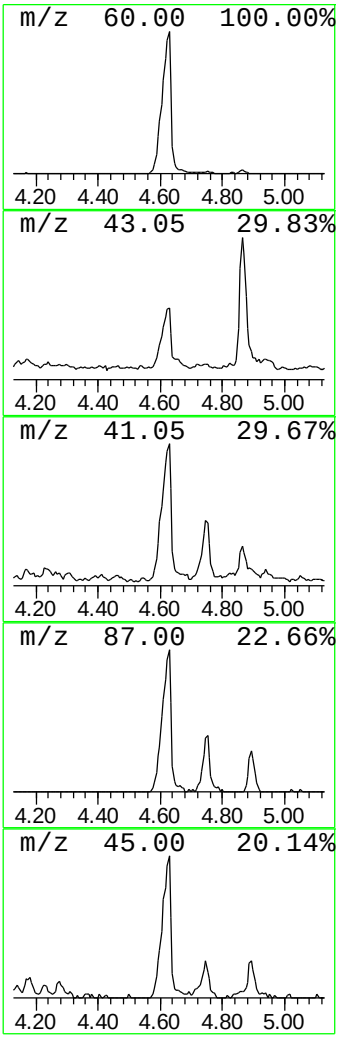
****

Peak Number 1 Butanoic acid, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	3.49 ng	408461	1,4-Dichlorobenzene-d4	7.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	78
2	Heptanoic acid	130	C7H14O2	000111-14-8	43
3	Pentanoic acid	102	C5H10O2	000109-52-4	38
4	1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	38
5	Urea, N-methyl-N-nitroso-	103	C2H5N3O2	000684-93-5	28





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Data File : BM018783.D
Acq On : 12 Feb 2019 21:29
Operator : JU/SJ
Sample : K1460-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-2-20190208

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

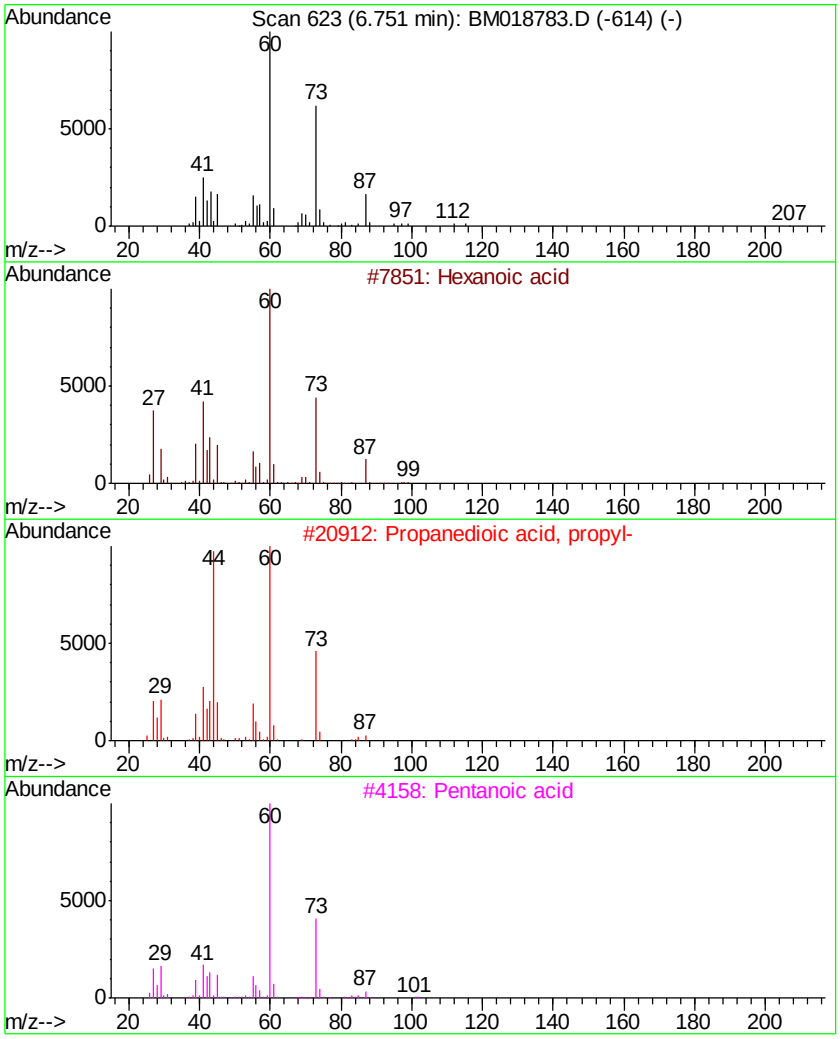
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

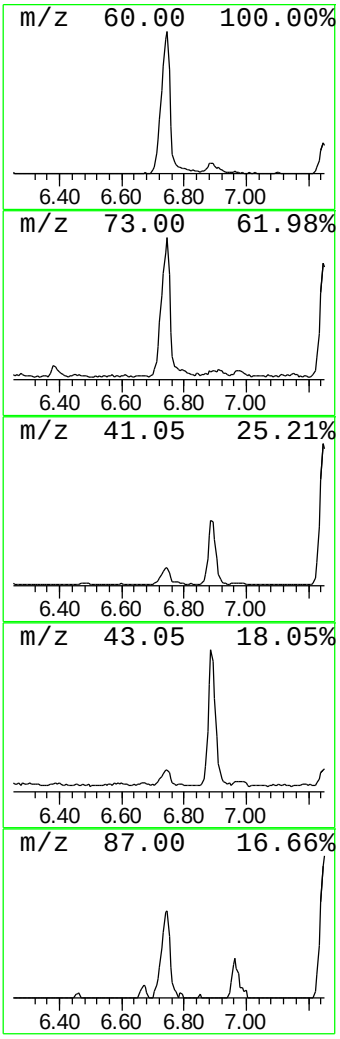
****

Peak Number 2 Hexanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	2.42 ng	283559	1,4-Dichlorobenzene-d4	7.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid	116	C6H12O2	000142-62-1	83
2	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	78
3	Pentanoic acid	102	C5H10O2	000109-52-4	64
4	Heptanoic acid	130	C7H14O2	000111-14-8	50
5	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	45





Library Search Compound Report

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Data File : BM018783.D
Acq On : 12 Feb 2019 21:29
Operator : JU/SJ
Sample : K1460-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-2-20190208

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

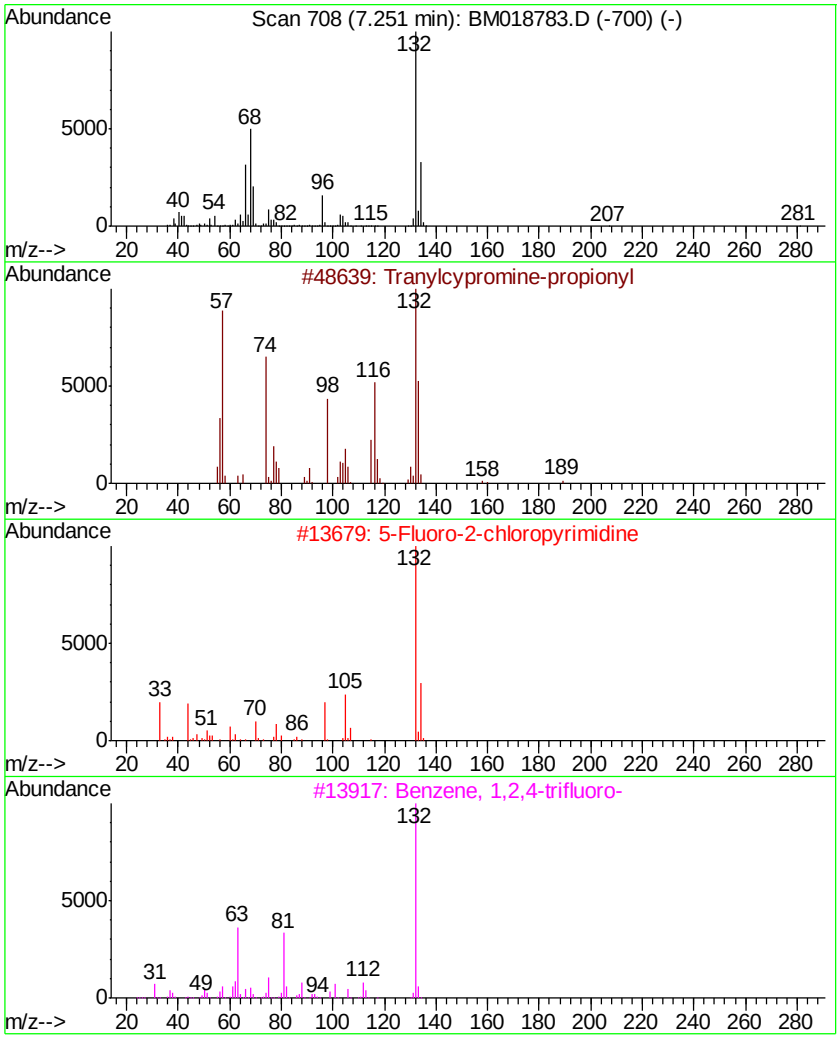
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

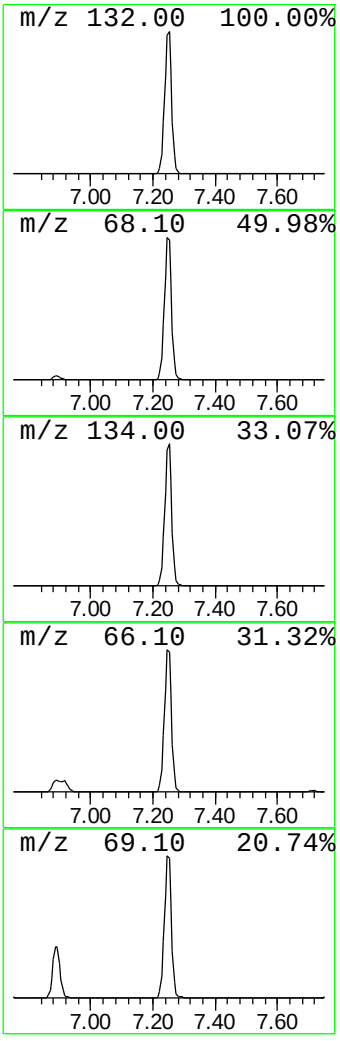
****

Peak Number 3 unknown7.25 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.25	93.31 ng	10926400	1,4-Dichlorobenzene-d4	7.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
4	Xenon	132	Xe	007440-63-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

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Operator : JU/SJ
Sample : K1460-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-2-20190208

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
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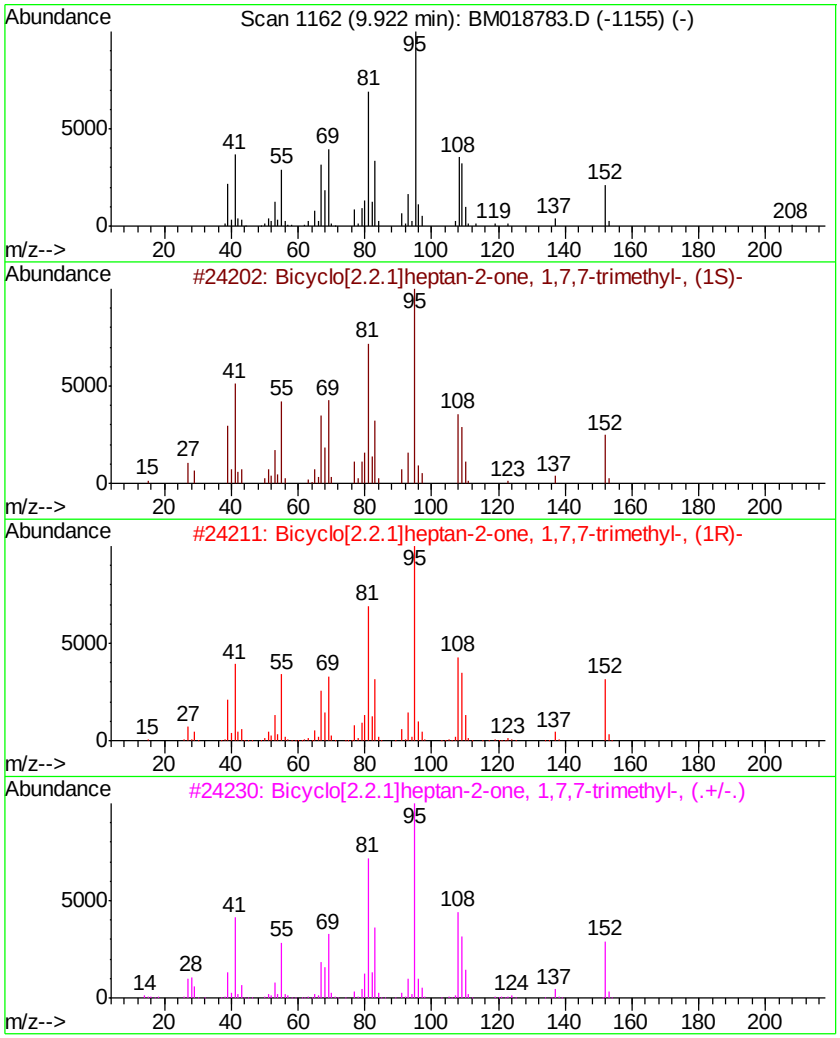
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

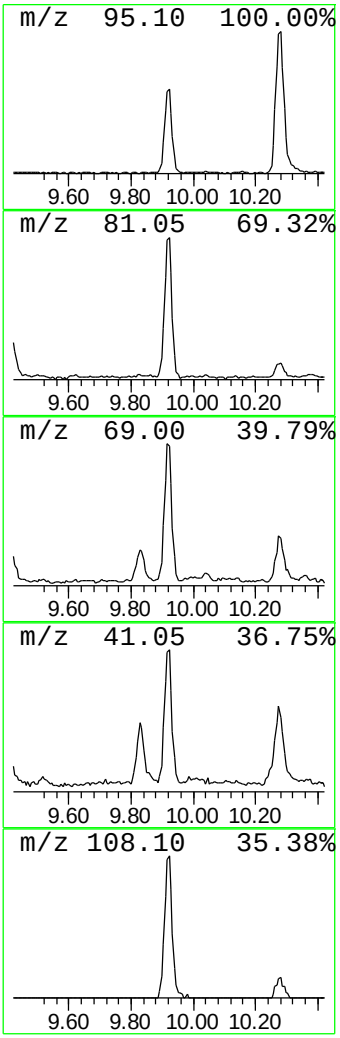
****

Peak Number 5 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.92	2.64 ng	418254	Naphthalene-d8	10.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	98
2	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-49-3	97
3	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	021368-68-3	97
4	Camphor	152	C10H16O	000076-22-2	95
5	5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	58





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021219\
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Acq On : 12 Feb 2019 21:29
Operator : JU/SJ
Sample : K1460-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-2-20190208

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

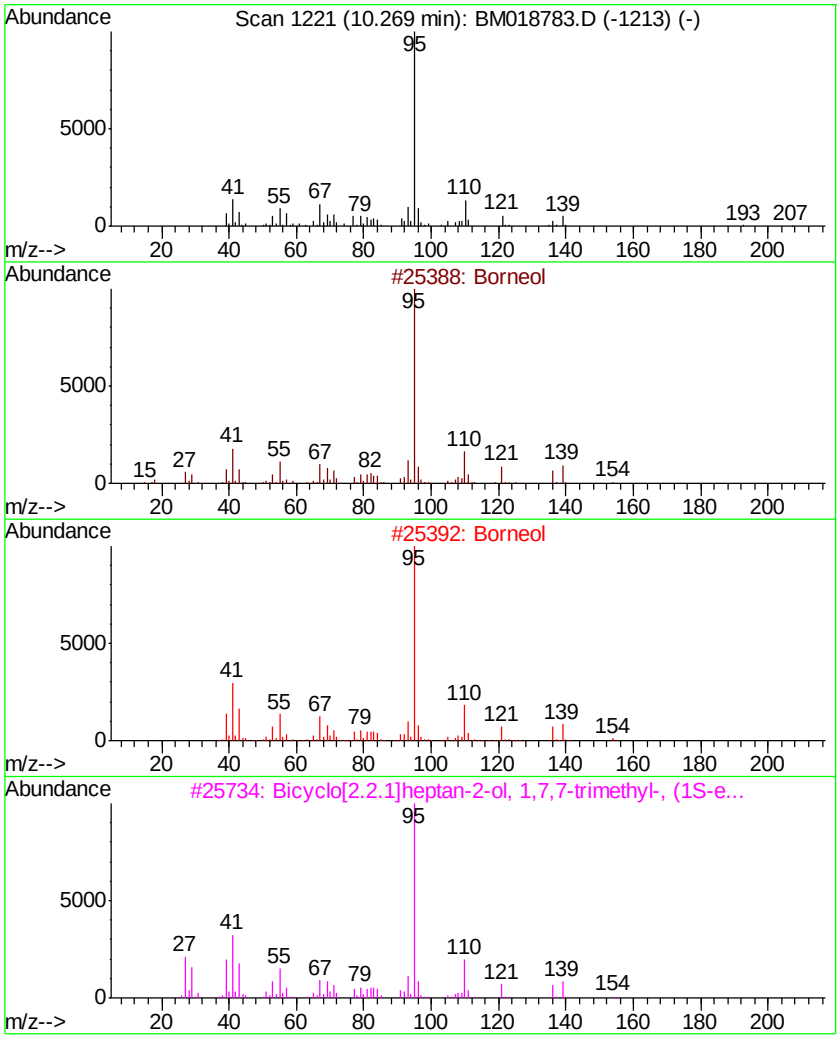
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

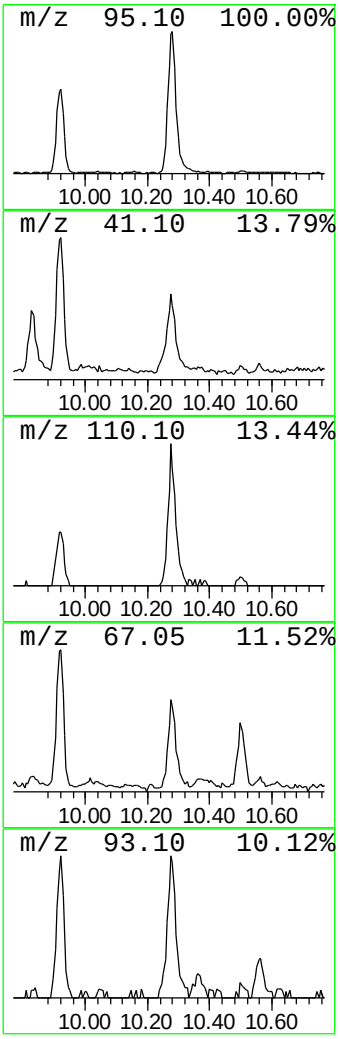
****

Peak Number 6 Borneol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.27	2.49 ng	395191	Naphthalene-d8	10.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Borneol	154	C10H18O	000507-70-0	90
2	Borneol	154	C10H18O	010385-78-1	83
3	Bicyclo[2.2.1]heptan-2-ol, 1,7,7...	154	C10H18O	000464-45-9	83
4	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	72
5	Cyclopropane, 2-(1,1-dimethyl-2-...	166	C12H22	074663-76-6	59





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021219\
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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-2-20190208

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

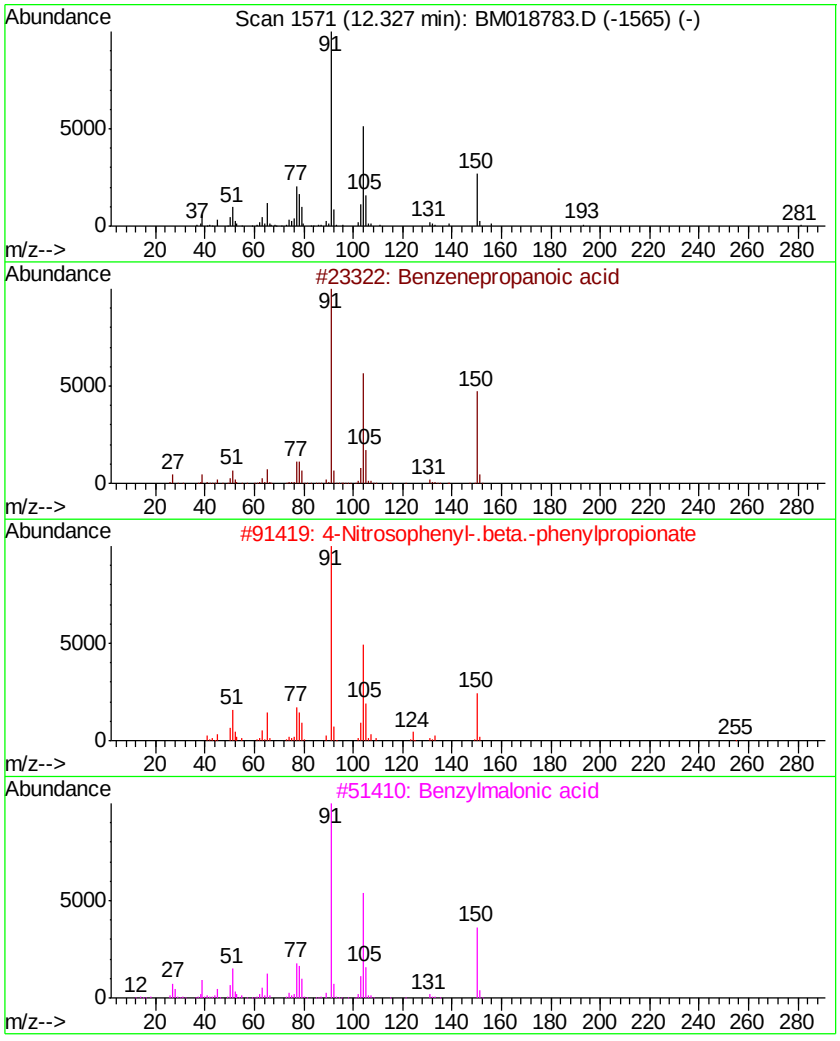
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

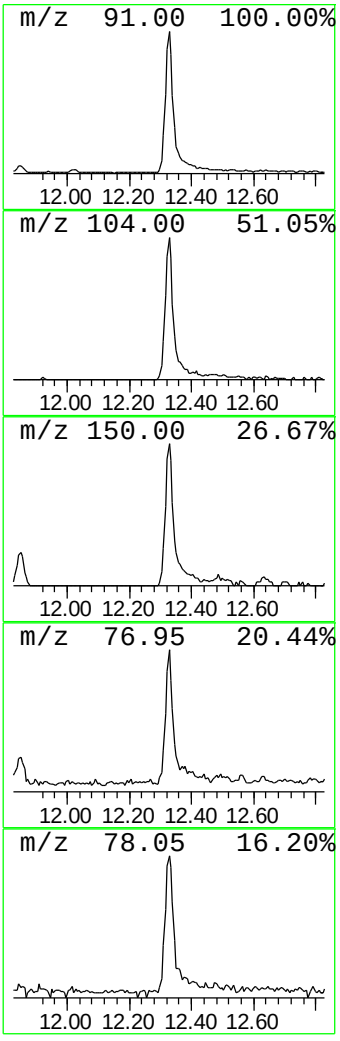
****

Peak Number 7 Benzenepropanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.33	2.16 ng	342736	Naphthalene-d8	10.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenepropanoic acid	150	C9H10O2	000501-52-0	90
2	4-Nitrosophenyl-.beta.-phenylpro...	255	C15H13NO3	1000129-40-0	90
3	Benzylmalonic acid	194	C10H10O4	000616-75-1	80
4	Benzene, 4-pentenyl-	146	C11H14	001075-74-7	53
5	Phenylethyl methacrylate	190	C12H14O2	003683-12-3	47





Library Search Compound Report

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ClientSampleId : MW-2-20190208

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

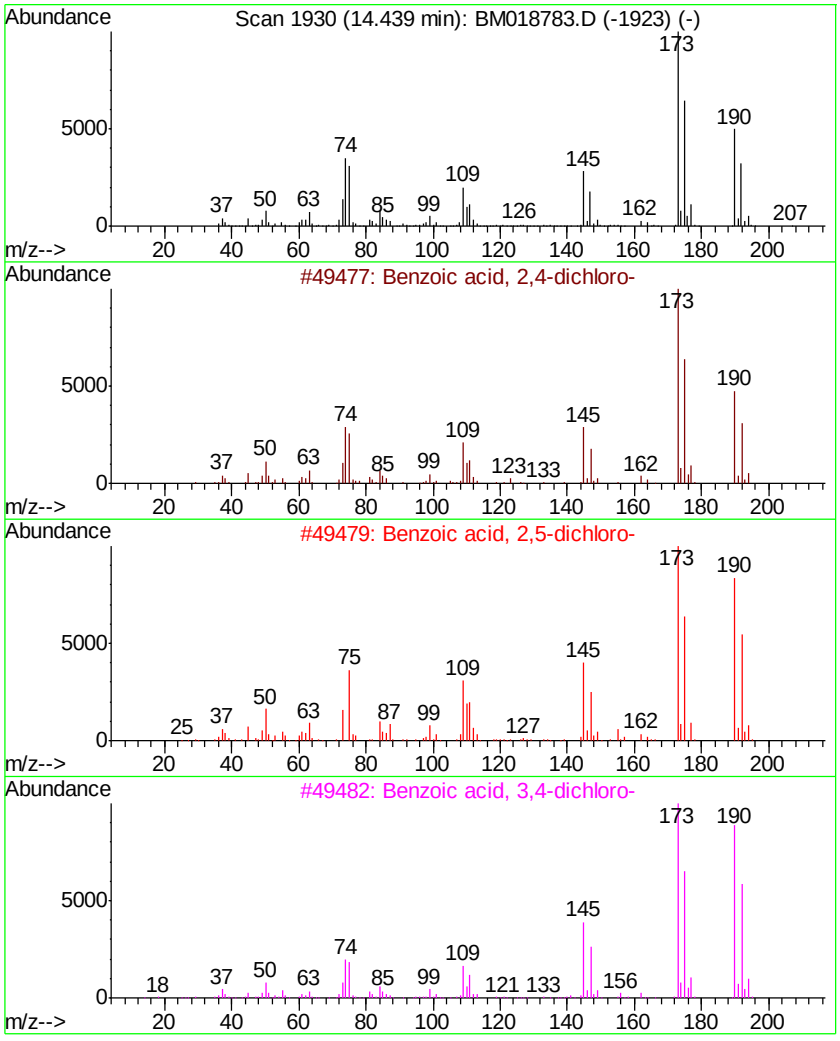
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

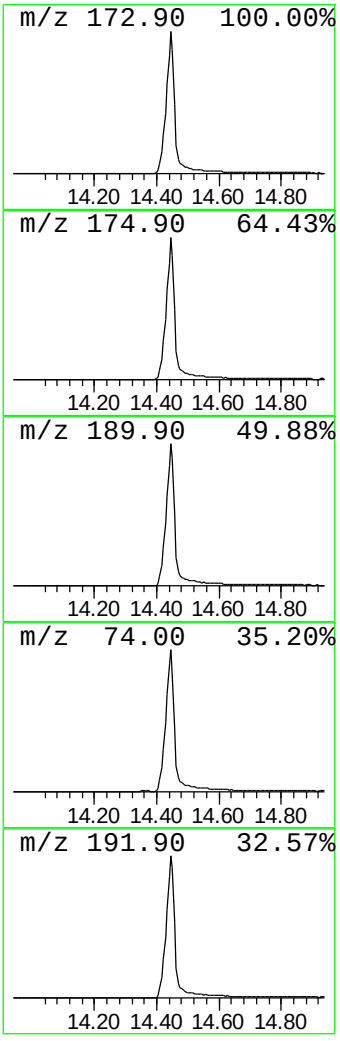
****

Peak Number 8 Benzoic acid, 2,4-dichloro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.44	41.32 ng	8773320	Acenaphthene-d10	14.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2,4-dichloro-	190	C7H4Cl2O2	000050-84-0	99
2	Benzoic acid, 2,5-dichloro-	190	C7H4Cl2O2	000050-79-3	97
3	Benzoic acid, 3,4-dichloro-	190	C7H4Cl2O2	000051-44-5	96
4	Benzoic acid, 2,6-dichloro-	190	C7H4Cl2O2	000050-30-6	95
5	Benzoic acid, 2,3-dichloro-	190	C7H4Cl2O2	000050-45-3	92





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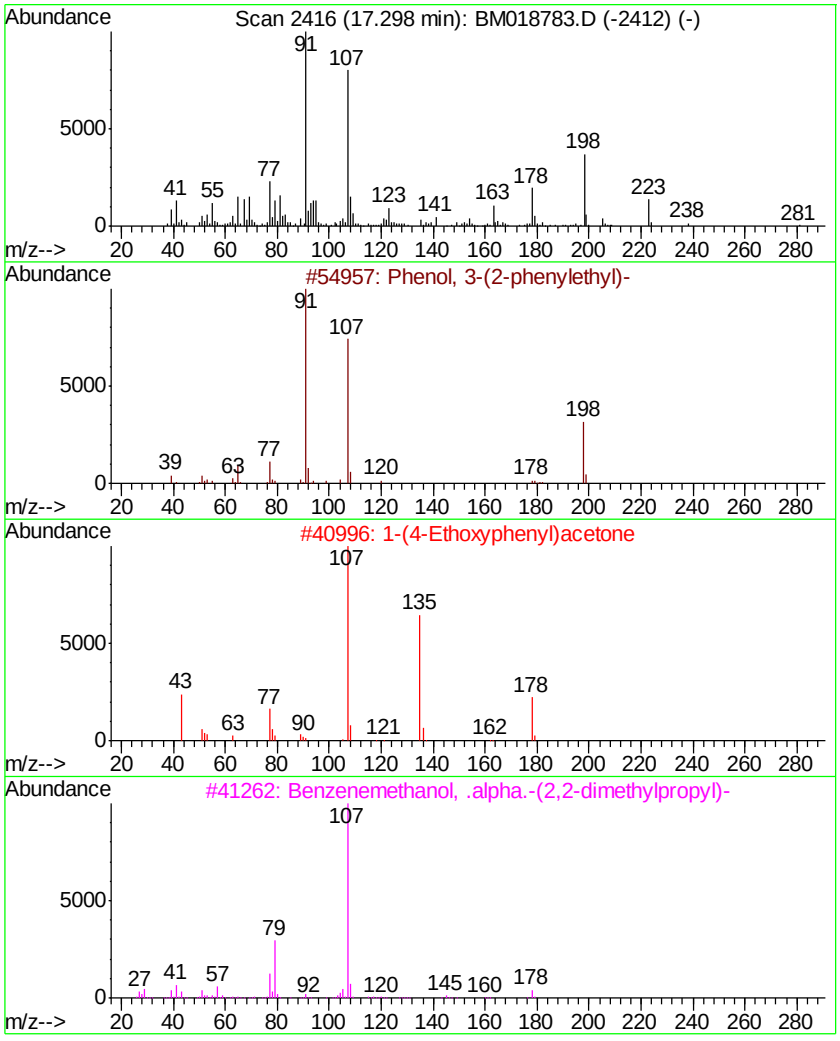
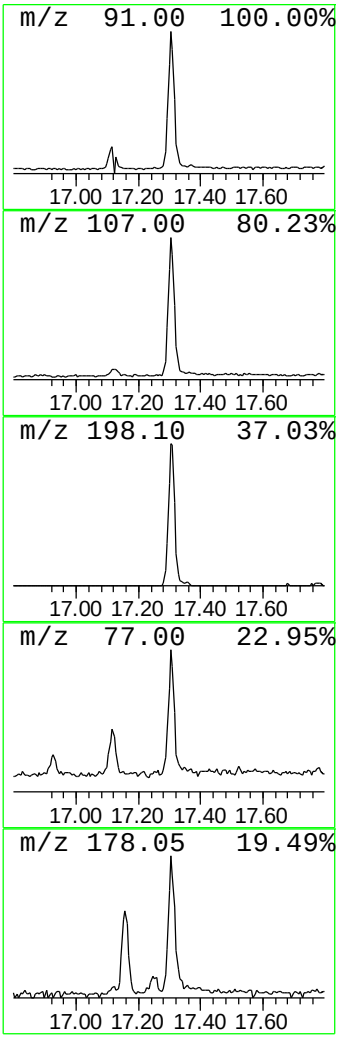
****

Peak Number 9 Phenol, 3-(2-phenylethyl)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.30	2.23 ng	580724	Phenanthrene-d10	17.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 3-(2-phenylethyl)-	198	C14H14O	033675-75-1	70
2	1-(4-Ethoxyphenyl)acetone	178	C11H14O2	144818-72-4	43
3	Benzenemethanol, .alpha.-(2,2-di...	178	C12H18O	062338-03-8	38
4	3-Benzyloxy-butyric acid, t-buty...	250	C15H22O3	116761-25-2	38
5	Phenol, 2-propyl-	136	C9H12O	000644-35-9	38





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
Butanoic acid, 3-...	4.63	3.5	ng	408461	1	7.71	2342080	20.0
Hexanoic acid	6.75	2.4	ng	283559	1	7.71	2342080	20.0
unknown7.25	7.25	93.3	ng	10926400	1	7.71	2342080	20.0
Bicyclo[2.2.1]hep...	9.92	2.6	ng	418254	2	10.50	3168740	20.0
Borneol	10.27	2.5	ng	395191	2	10.50	3168740	20.0
Benzenepropanoic ...	12.33	2.2	ng	342736	2	10.50	3168740	20.0
Benzoic acid, 2,4...	14.44	41.3	ng	8773320	3	14.36	4246070	20.0
Phenol, 3-(2-phen...	17.30	2.2	ng	580724	4	17.12	5214540	20.0