LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030921\
Data File : BM029063.D
Acq On : 10 Mar 2021 01:34
Operator : CG/JU
Sample : M1603-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 33-NORTH

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-BM022321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029063.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.152	193	198	202	rBV	18866	25807	4.48%	1.236%
2	4.193	202	205	218	rVB2	6230	13163	2.29%	0.630%
3	4.769	297	303	313	rVB	81549	108500	18.85%	5.196%
4	5.246	379	384	394	rVB	24366	38032	6.61%	1.821%
5	5.722	458	465	475	rBV2	7631	15087	2.62%	0.723%
6	6.869	654	660	674	rVB	119246	193894	33.68%	9.286%
7	7.669	790	796	802	rBV	57231	85946	14.93%	4.116%
8	8.845	990	996	1006	rBV	94138	155454	27.00%	7.445%
9	8.998	1017	1022	1031	rVB2	7853	12770	2.22%	0.612%
10	10.463	1265	1271	1277	rVB	67770	104675	18.18%	5.013%
11	10.563	1283	1288	1299	rVB2	10274	16450	2.86%	0.788%
12	12.033	1533	1538	1543	rVB2	7490	10506	1.82%	0.503%
13	12.951	1687	1694	1702	rBV	228046	321091	55.78%	15.378%
14	13.298	1748	1753	1758	rBV	22647	31042	5.39%	1.487%
15	13.804	1835	1839	1844	rVB	9999	12349	2.15%	0.591%
16	14.210	1904	1908	1916	rBV2	14198	21958	3.81%	1.052%
17	14.339	1925	1930	1935	rBV2	87431	123125	21.39%	5.897%
18	15.345	2097	2101	2106	rBV	17984	21478	3.73%	1.029%
19	15.974	2204	2208	2215	rBV9	7797	20572	3.57%	0.985%
20	16.063	2219	2223	2226	rVV3	8443	11673	2.03%	0.559%
21	16.215	2245	2249	2255	rBV7	9670	17862	3.10%	0.855%
22	17.009	2382	2384	2390	rBV4	11904	15030	2.61%	0.720%
23	17.086	2393	2397	2402	rBV	96207	135826	23.59%	6.505%
24	19.721	2841	2845	2850	rVB	504133	575672	100.00%	27.571%

Sum of corrected areas: 2087962

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Instrument :
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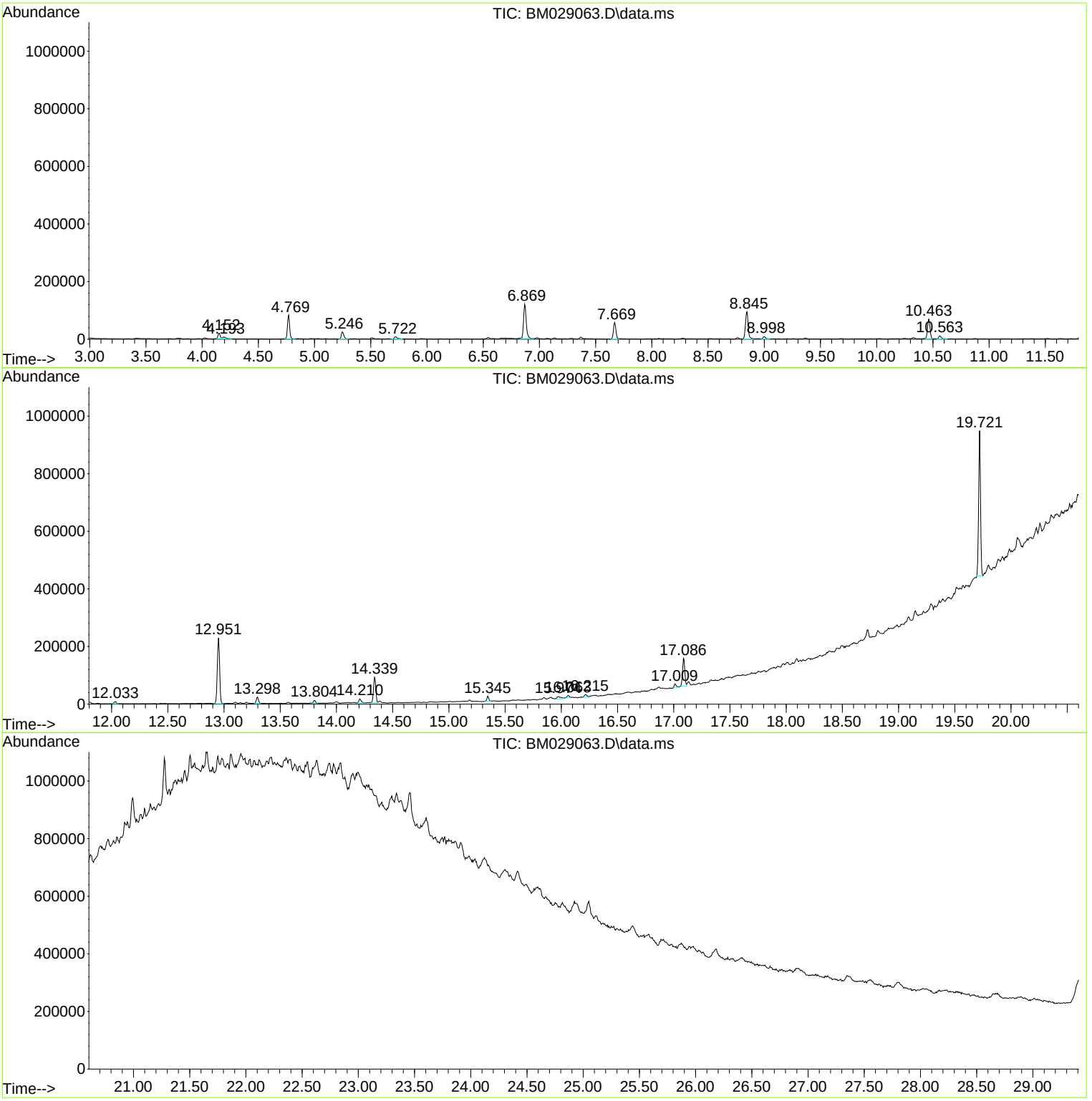
33-NORTH

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.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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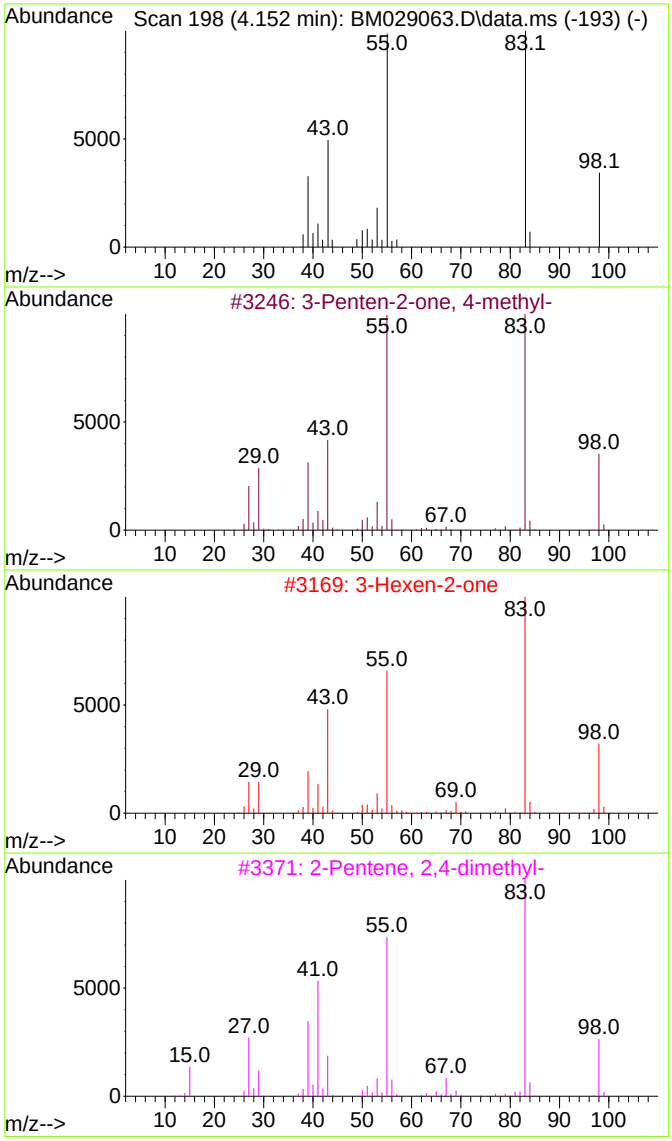
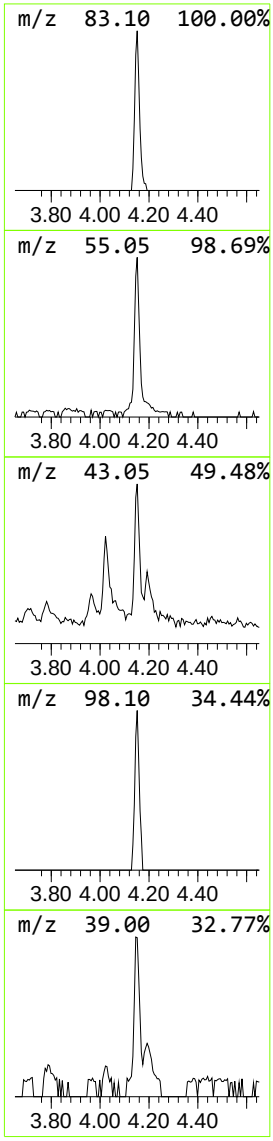
Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.152	6.01 ng	25807	1,4-Dichlorobenzene-d4	7.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	87
2	3-Hexen-2-one	98	C6H10O	000763-93-9	86
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
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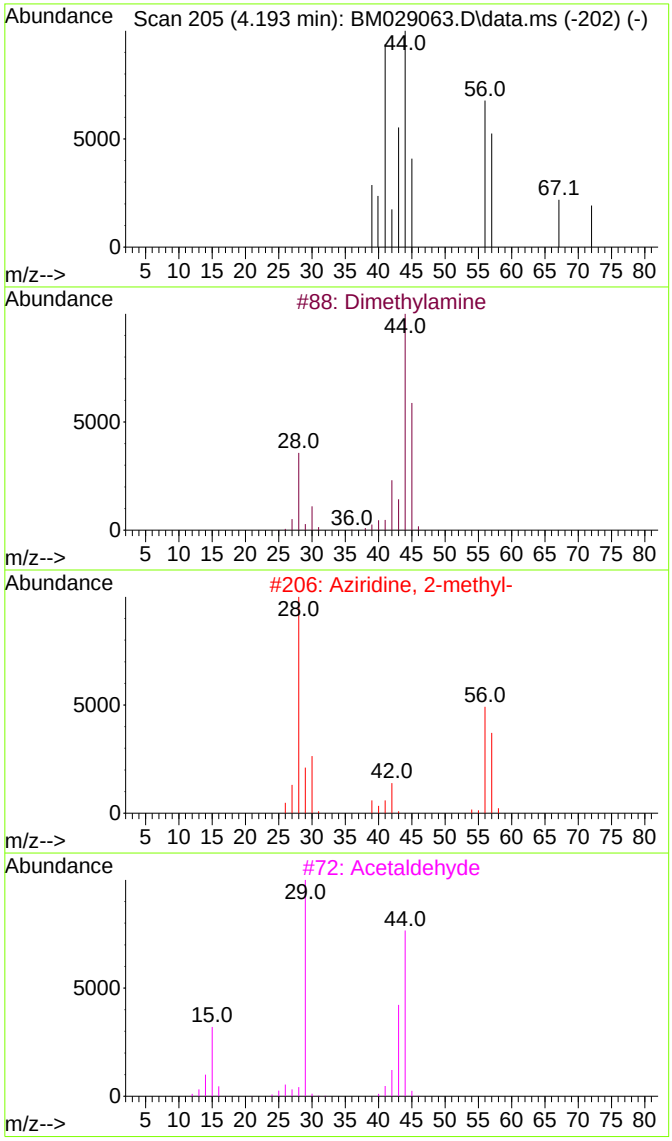
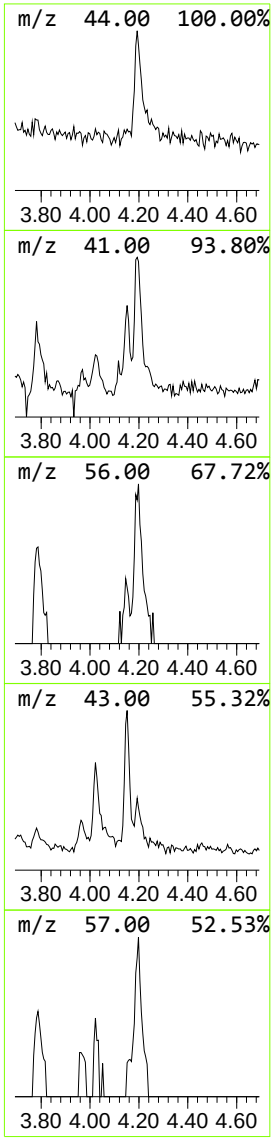
Peak Number 2 unknown4.193 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.193	3.06 ng	13163	1,4-Dichlorobenzene-d4	7.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethylamine	45	C2H7N	000124-40-3	9
2	Aziridine, 2-methyl-	57	C3H7N	000075-55-8	9
3	Acetaldehyde	44	C2H4O	000075-07-0	7
4	2,3-Epoxybutane	72	C4H8O	003266-23-7	7
5	2-Butene, (E)-	56	C4H8	000624-64-6	5





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
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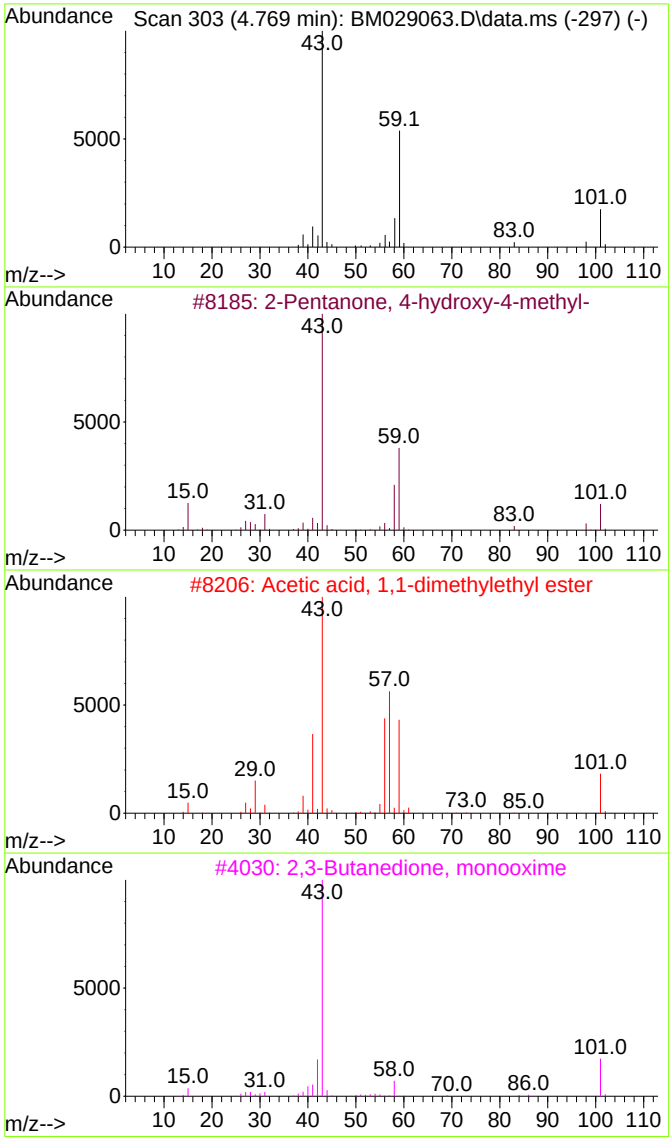
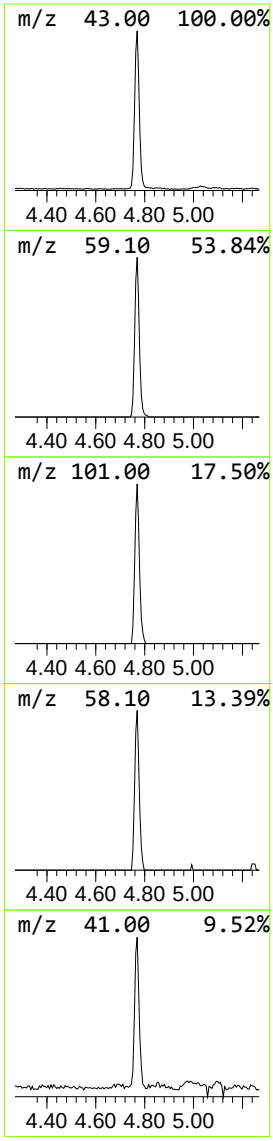
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.769	25.25 ng	108500	1,4-Dichlorobenzene-d4	7.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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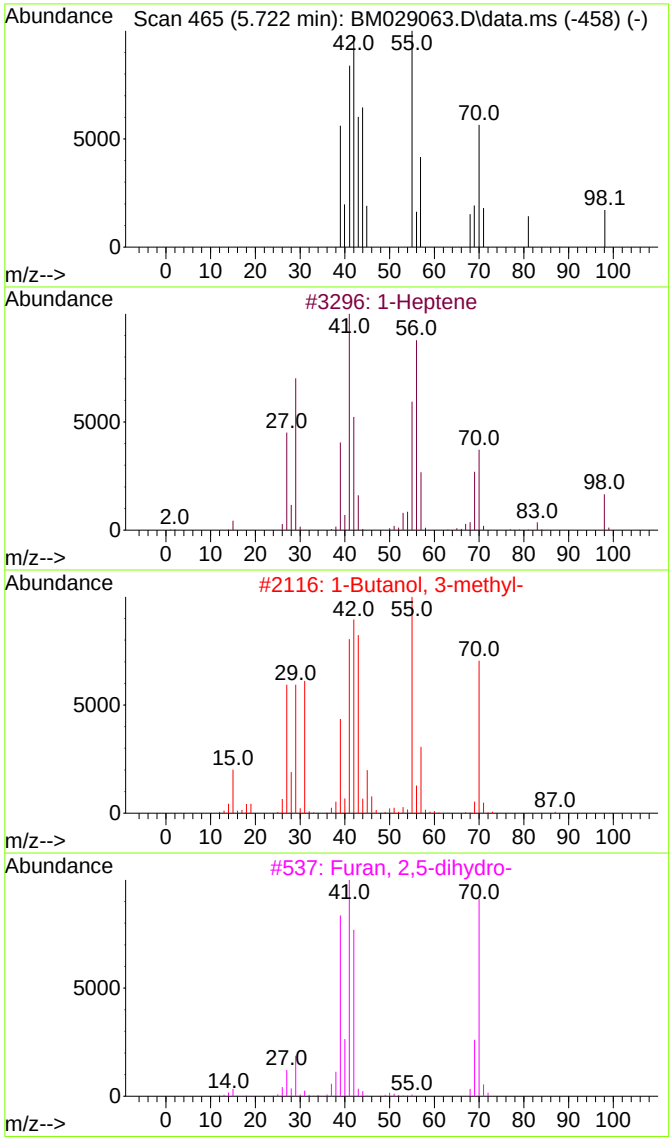
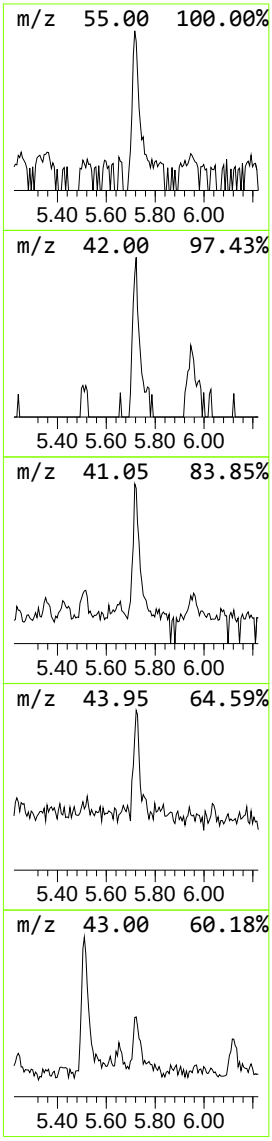
Peak Number 4 1-Heptene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.722	3.51 ng	15087	1,4-Dichlorobenzene-d4	7.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptene	98	C7H14	000592-76-7	53
2	1-Butanol, 3-methyl-	88	C5H12O	000123-51-3	47
3	Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	43
4	Heptanal	114	C7H14O	000111-71-7	43
5	2-Hexenal, (E)-	98	C6H10O	006728-26-3	38





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Sample : M1603-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
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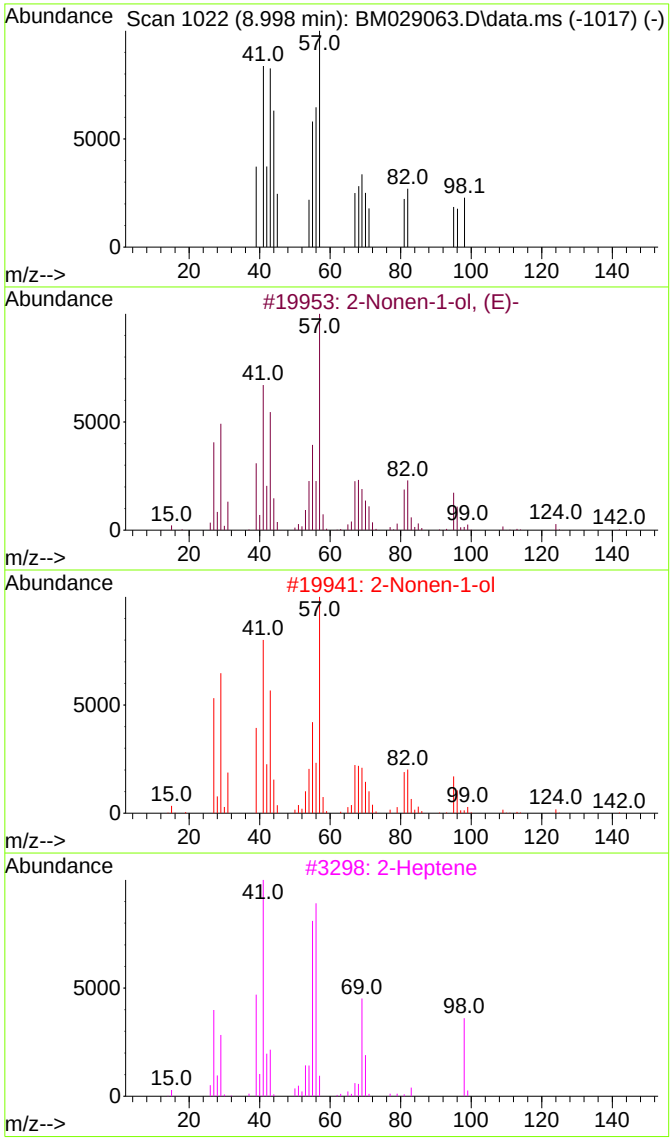
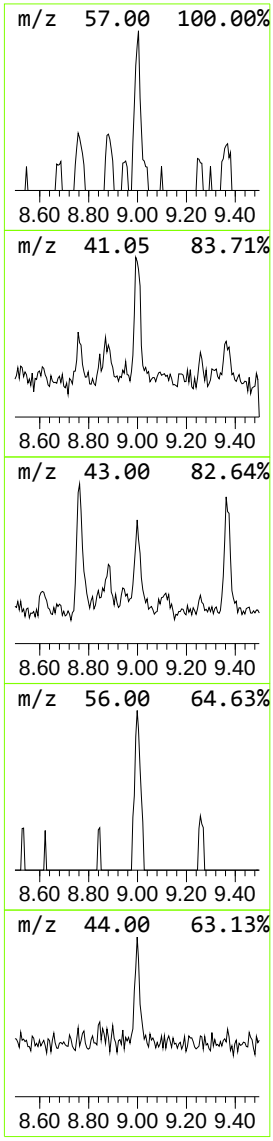
Peak Number 5 unknown8.998 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.998	2.97 ng	12770	1,4-Dichlorobenzene-d4	7.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonen-1-ol, (E)-	142	C9H18O	031502-14-4	47
2	2-Nonen-1-ol	142	C9H18O	022104-79-6	43
3	2-Heptene	98	C7H14	000592-77-8	25
4	(Z)-2-Heptene	98	C7H14	006443-92-1	25
5	2-Hepten-1-ol, (E)-	114	C7H14O	033467-76-4	25





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Misc :
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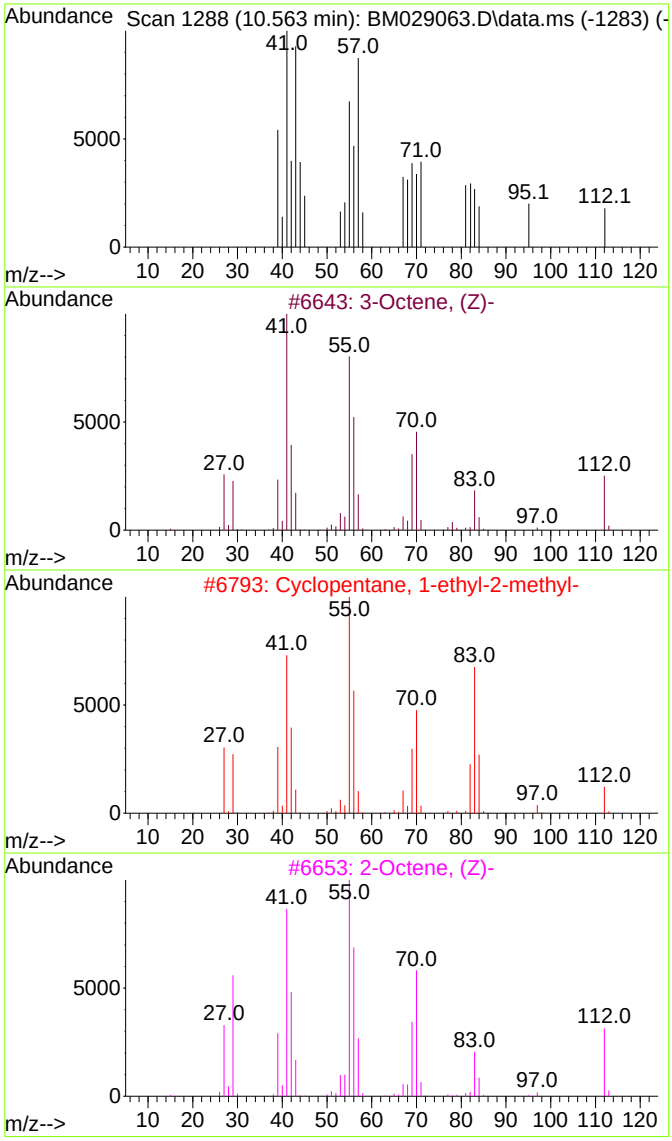
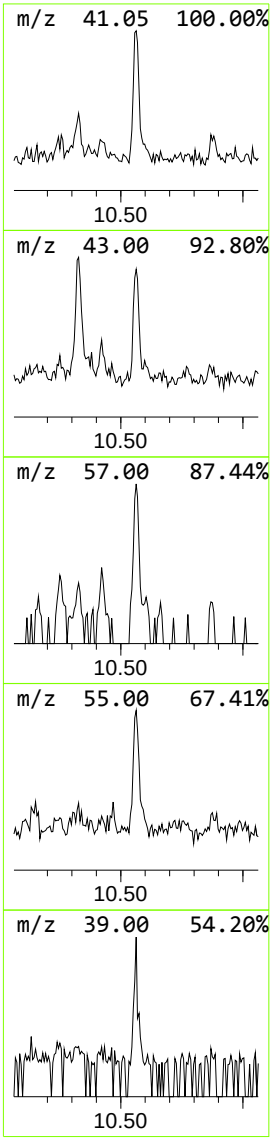
Peak Number 6 unknown10.563 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.563	3.14 ng	16450	Naphthalene-d8	10.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octene, (Z)-	112	C8H16	014850-22-7	43
2	Cyclopentane, 1-ethyl-2-methyl-	112	C8H16	003726-46-3	43
3	2-Octene, (Z)-	112	C8H16	007642-04-8	38
4	2-Octene	112	C8H16	000111-67-1	35
5	1-Dodecene	168	C12H24	000112-41-4	35





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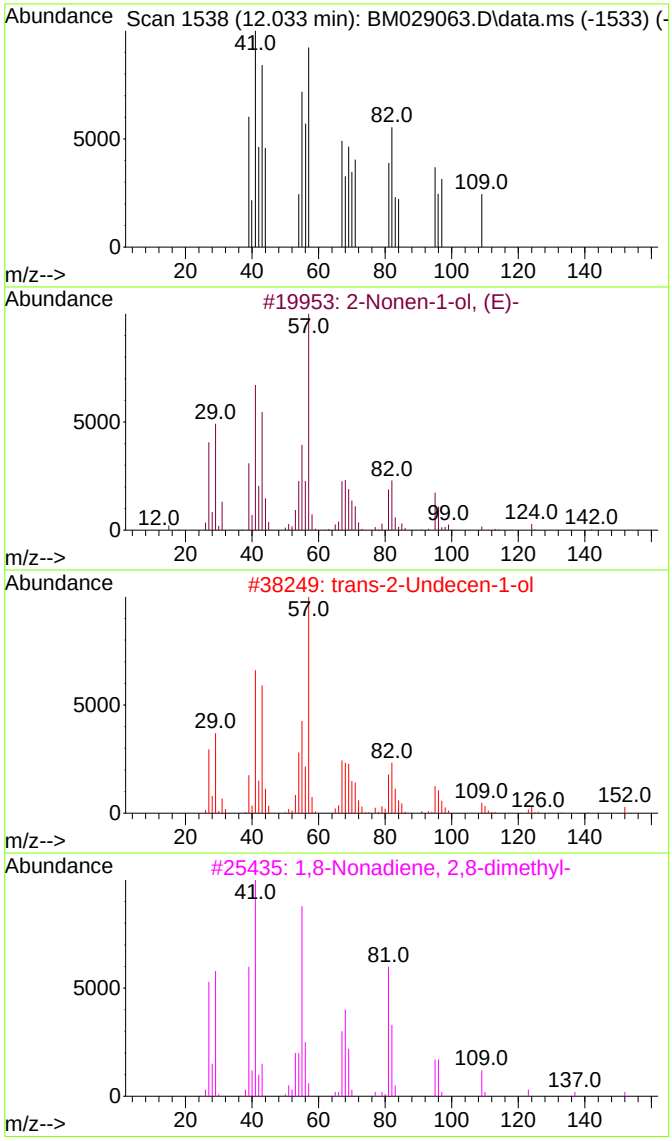
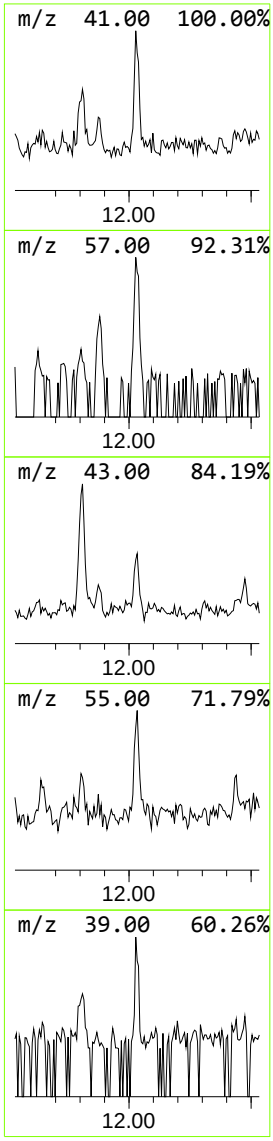
Peak Number 7 unknown12.033 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.033	2.01 ng	10506	Naphthalene-d8	10.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonen-1-ol, (E)-	142	C9H18O	031502-14-4	47
2	trans-2-Undecen-1-ol	170	C11H22O	075039-84-8	38
3	1,8-Nonadiene, 2,8-dimethyl-	152	C11H20	020054-25-5	32
4	3-Decyn-2-ol	154	C10H18O	069668-93-5	25
5	2-Hexen-1-ol, (E)-	100	C6H12O	000928-95-0	23





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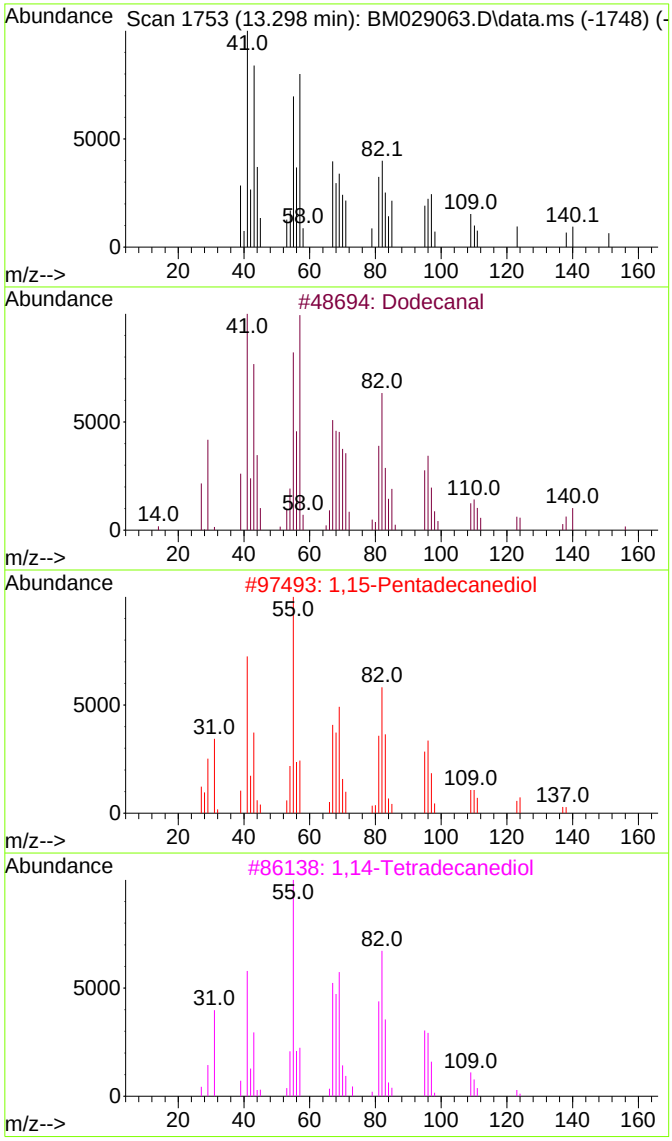
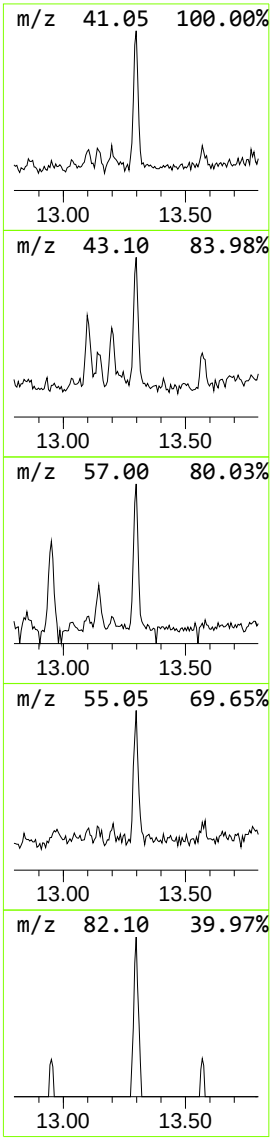
Peak Number 8 Dodecanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.298	5.04 ng	31042	Acenaphthene-d10	14.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanal	184	C12H24O	000112-54-9	83
2	1,15-Pentadecanediol	244	C15H32O2	014722-40-8	64
3	1,14-Tetradecanediol	230	C14H30O2	019812-64-7	58
4	cis-9-Tetradecen-1-ol	212	C14H28O	035153-15-2	53
5	13-Oxabicyclo[10.1.0]tridecane	182	C12H22O	000286-99-7	53





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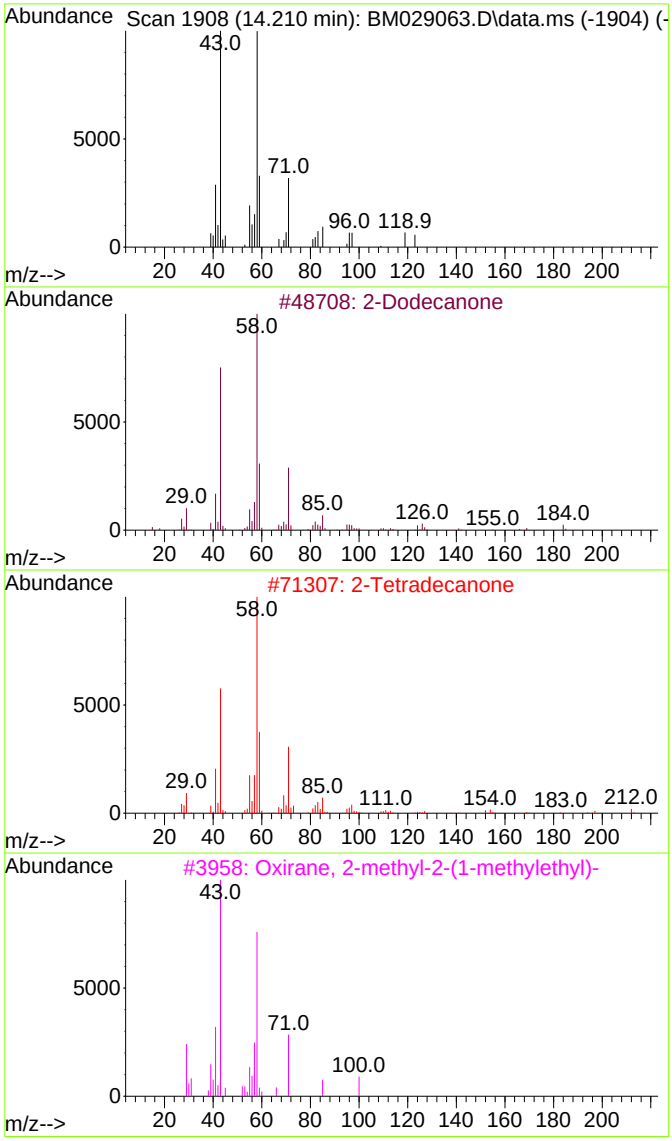
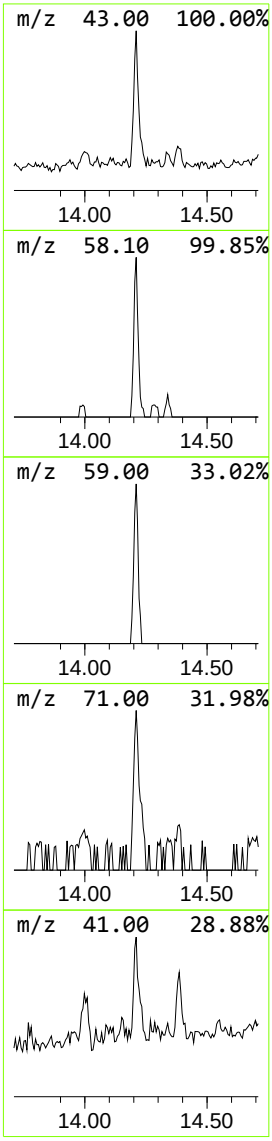
Peak Number 9 2-Dodecanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.210	3.57 ng	21958	Acenaphthene-d10	14.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Dodecanone	184	C12H24O	006175-49-1	72
2	2-Tetradecanone	212	C14H28O	002345-27-9	56
3	Oxirane, 2-methyl-2-(1-methyleth...	100	C6H12O	072221-03-5	53
4	Pentanal, 2-methyl-	100	C6H12O	000123-15-9	40
5	Butanimidamide	86	C4H10N2	000107-90-4	40





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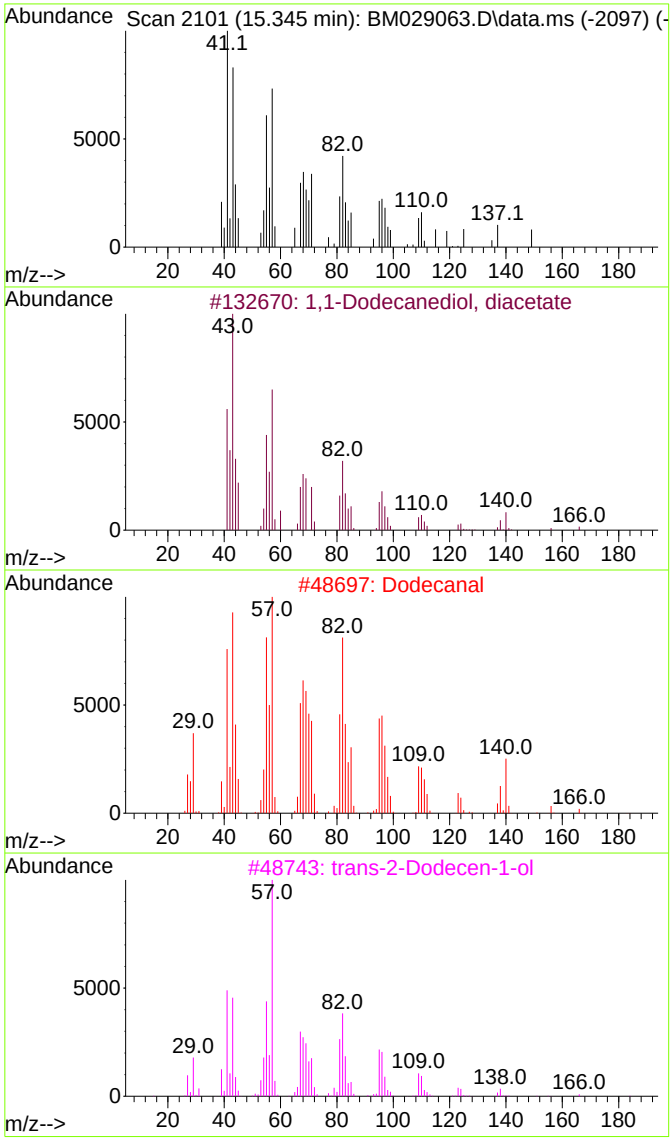
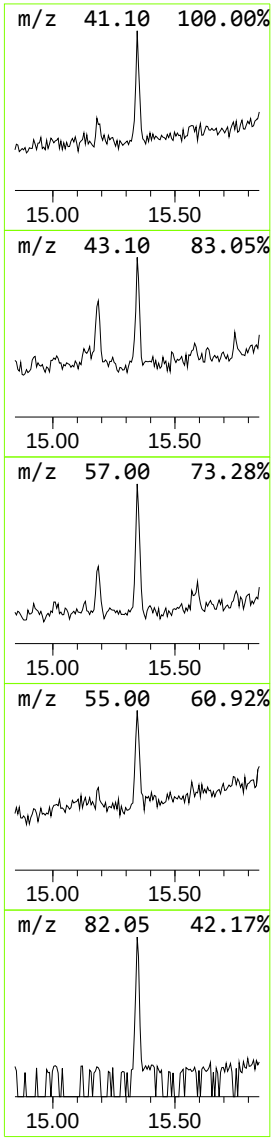
Peak Number 10 1,1-Dodecanediol, diacetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.345	3.49 ng	21478	Acenaphthene-d10	14.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1-Dodecanediol, diacetate	286	C16H30O4	056438-07-4	87
2	Dodecanal	184	C12H24O	000112-54-9	83
3	trans-2-Dodecen-1-ol	184	C12H24O	069064-37-5	64
4	E-2-Tetradecen-1-ol	212	C14H28O	1000130-83-7	64
5	1,12-Dodecanediol	202	C12H26O2	005675-51-4	62





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Data File : BM029063.D
Acq On : 10 Mar 2021 01:34
Operator : CG/JU
Sample : M1603-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
33-NORTH

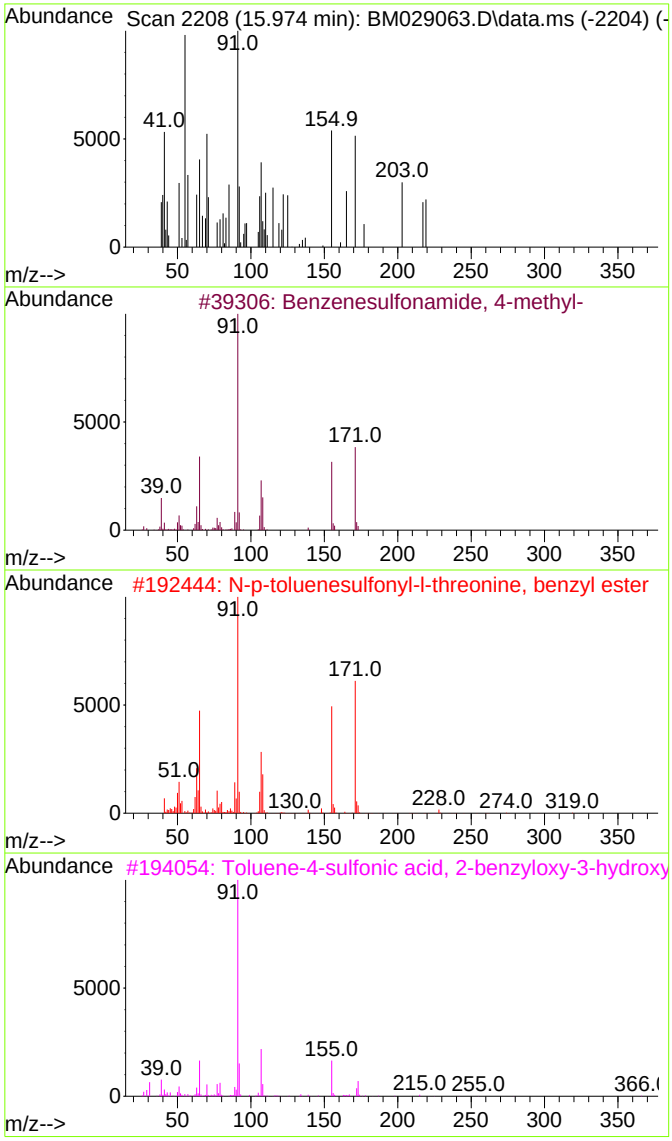
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

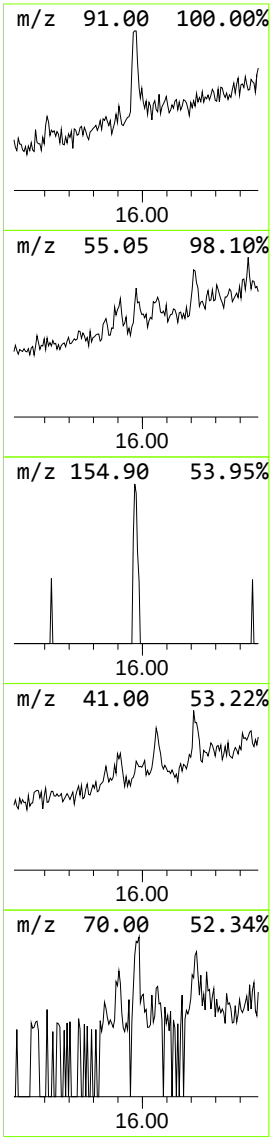
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Benzenesulfonamide, 4-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.974	3.03 ng	20572	Phenanthrene-d10	17.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	53
2	N-p-toluenesulfonyl-l-threonine,...	363	C18H21NO5S	1000130-34-4	42
3	Toluene-4-sulfonic acid, 2-benzy...	366	C18H22O6S	118653-93-3	38
4	Tricyclo[2.1.1.0(5,6)]hexane-2-c...	275	C14H13NO3S	103495-50-7	32
5	Oxiraneethanol, .beta.-(phenylme...	348	C18H20O5S	118653-94-4	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030921\
Data File : BM029063.D
Acq On : 10 Mar 2021 01:34
Operator : CG/JU
Sample : M1603-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 33-NORTH

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.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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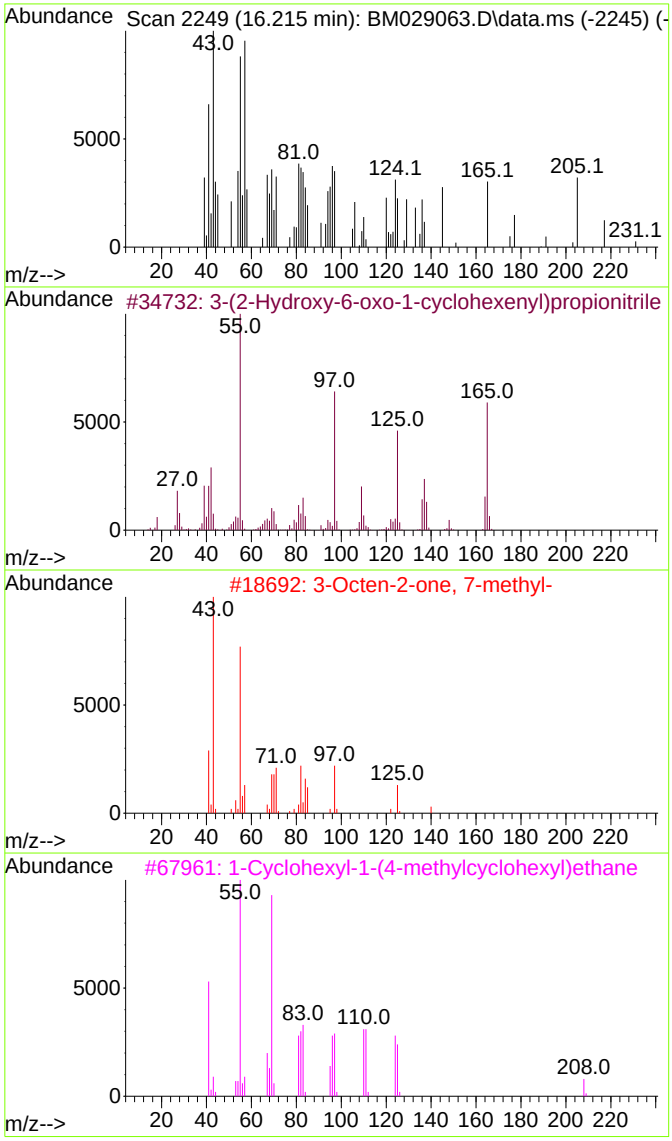
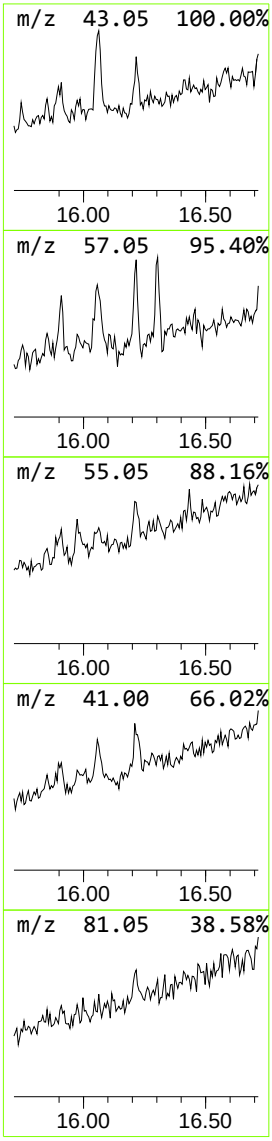
Peak Number 12 unknown16.215 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.215	2.63 ng	17862	Phenanthrene-d10	17.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(2-Hydroxy-6-oxo-1-cyclohexeny...	165	C9H11NO2	057943-19-8	18
2	3-Octen-2-one, 7-methyl-	140	C9H16O	033046-81-0	10
3	1-Cyclohexyl-1-(4-methylcyclohex...	208	C15H28	002027-12-5	10
4	Cyclohexane, (2,2-dimethylcyclop...	180	C13H24	061142-23-2	10
5	Histamine, N-t-butoxycarbonyl-2,...	563	C28H33N7O6	1000129-62-8	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030921\
Data File : BM029063.D
Acq On : 10 Mar 2021 01:34
Operator : CG/JU
Sample : M1603-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 33-NORTH

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.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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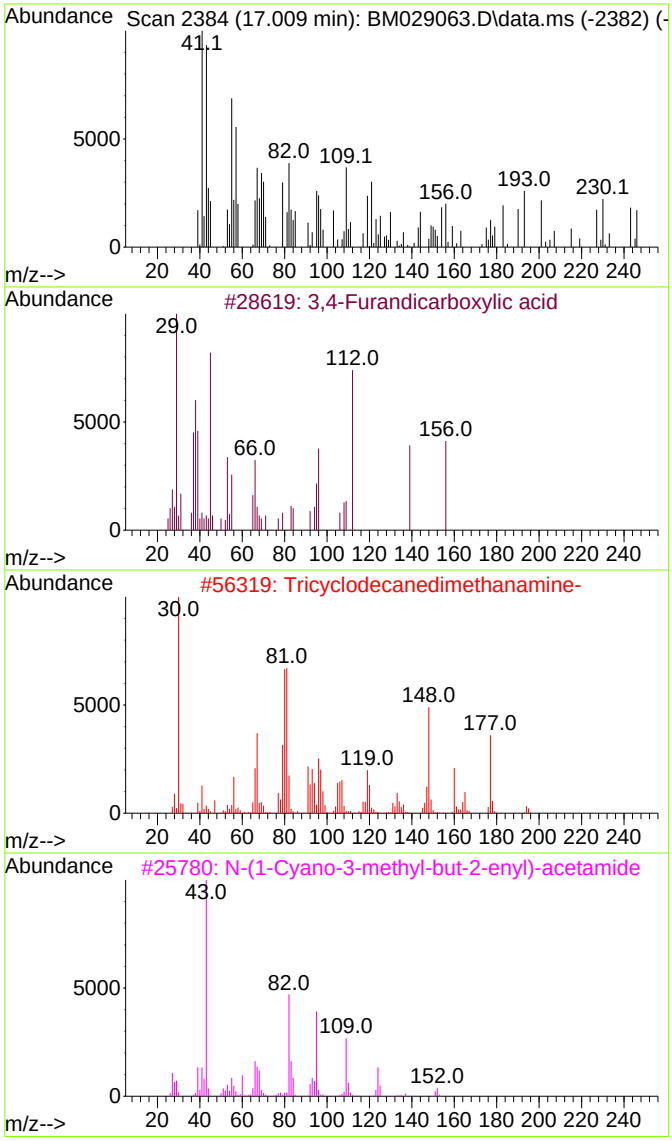
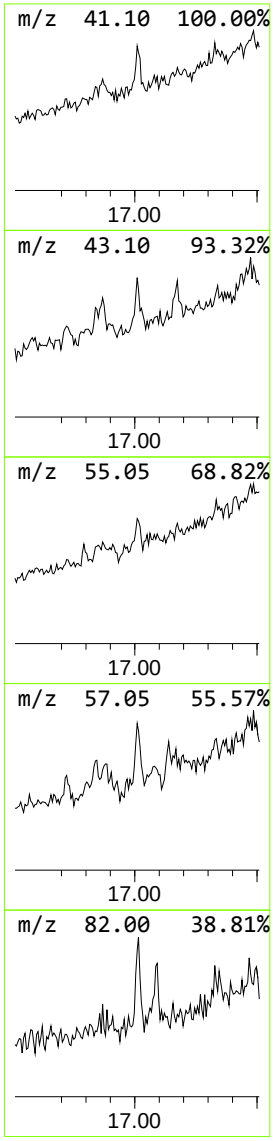
Peak Number 13 unknown17.009 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.009	2.21 ng	15030	Phenanthrene-d10	17.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Furandicarboxylic acid	156	C6H4O5	003387-26-6	32
2	Tricyclodecanedimethanamine-	194	C12H22N2	026655-37-8	17
3	N-(1-Cyano-3-methyl-but-2-enyl)-...	152	C8H12N2O	1000192-62-7	16
4	Imidazole, 1,4-dimethyl-5-nitro-	141	C5H7N3O2	057658-79-4	14
5	2-Nonynoic acid, ethyl ester	182	C11H18O2	010031-92-2	12





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030921\
Data File : BM029063.D
Acq On : 10 Mar 2021 01:34
Operator : CG/JU
Sample : M1603-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 33-NORTH

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
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
3-Penten-2-one,...	4.152	6.0	ng	25807	1	7.669	85946	20.0
unknown4.193	4.193	3.1	ng	13163	1	7.669	85946	20.0
2-Pentanone, 4-...	4.769	25.3	ng	108500	1	7.669	85946	20.0
1-Heptene	5.722	3.5	ng	15087	1	7.669	85946	20.0
unknown8.998	8.998	3.0	ng	12770	1	7.669	85946	20.0
unknown10.563	10.563	3.1	ng	16450	2	10.463	104675	20.0
unknown12.033	12.033	2.0	ng	10506	2	10.463	104675	20.0
Dodecanal	13.298	5.0	ng	31042	3	14.339	123125	20.0
2-Dodecanone	14.210	3.6	ng	21958	3	14.339	123125	20.0
1,1-Dodecanedio...	15.345	3.5	ng	21478	3	14.339	123125	20.0
Benzenesulfonam...	15.974	3.0	ng	20572	4	17.086	135826	20.0
unknown16.215	16.215	2.6	ng	17862	4	17.086	135826	20.0
unknown17.009	17.009	2.2	ng	15030	4	17.086	135826	20.0