LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112621\
Data File : BM033277.D
Acq On : 26 Nov 2021 22:28
Operator : CG/JU
Sample : M4803-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
261-262

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-BM112421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM033277.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.313	450	506	509	rVB3	29264753	432783598	100.00%	70.861%
2	8.207	820	828	844	rVB	6021497	10453745	2.42%	1.712%
3	9.107	938	981	986	rBV2	6302514	42711656	9.87%	6.993%
4	10.260	1136	1177	1181	rBV	2117037	13625209	3.15%	2.231%
5	10.554	1214	1227	1245	rBV	3955594	9379631	2.17%	1.536%
6	13.184	1664	1674	1683	rBV	4256487	7658613	1.77%	1.254%
7	13.983	1805	1810	1815	rBV2	3970449	6437365	1.49%	1.054%
8	14.301	1859	1864	1869	rBV5	2411698	5109450	1.18%	0.837%
9	14.389	1875	1879	1885	rVB	6254210	9419429	2.18%	1.542%
10	14.525	1897	1902	1905	rBV2	3022323	5441297	1.26%	0.891%
11	15.348	2038	2042	2046	rBV2	4638424	6751599	1.56%	1.105%
12	16.295	2197	2203	2208	rBV2	8921445	17870369	4.13%	2.926%
13	24.453	3582	3590	3596	rBV2	1746178	4772276	1.10%	0.781%
14	24.795	3642	3648	3656	rVB3	2758811	7650782	1.77%	1.253%
15	24.877	3656	3662	3672	rVB	2593264	5998865	1.39%	0.982%
16	25.000	3677	3683	3697	rVB	1986822	5216488	1.21%	0.854%
17	27.024	4013	4027	4035	rBV2	1159526	5255500	1.21%	0.861%
18	27.677	4129	4138	4155	rVB	2335571	8198386	1.89%	1.342%
19	27.877	4163	4172	4184	rVB	1863160	6015090	1.39%	0.985%

Sum of corrected areas: 610749348

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Misc :
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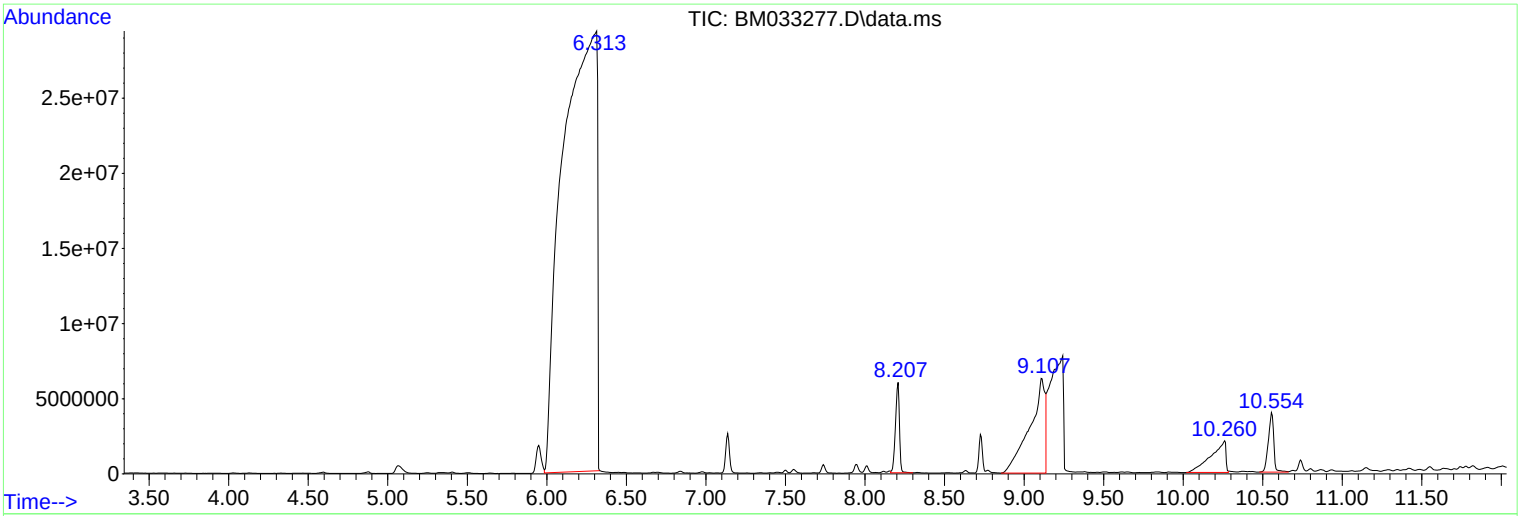
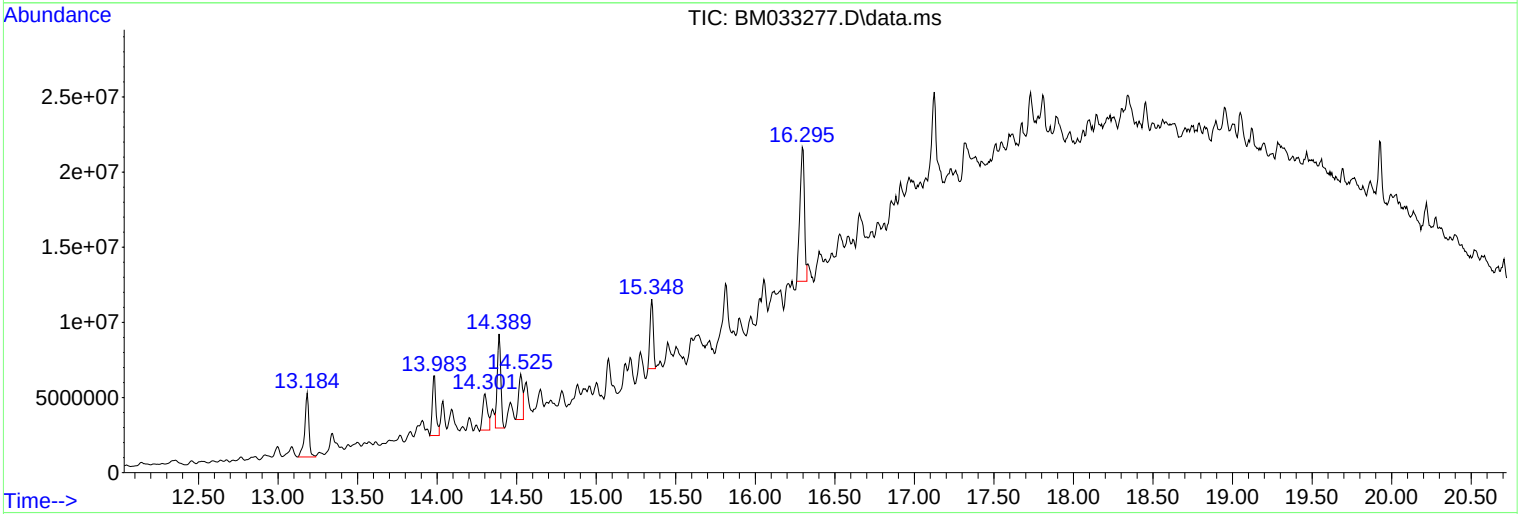
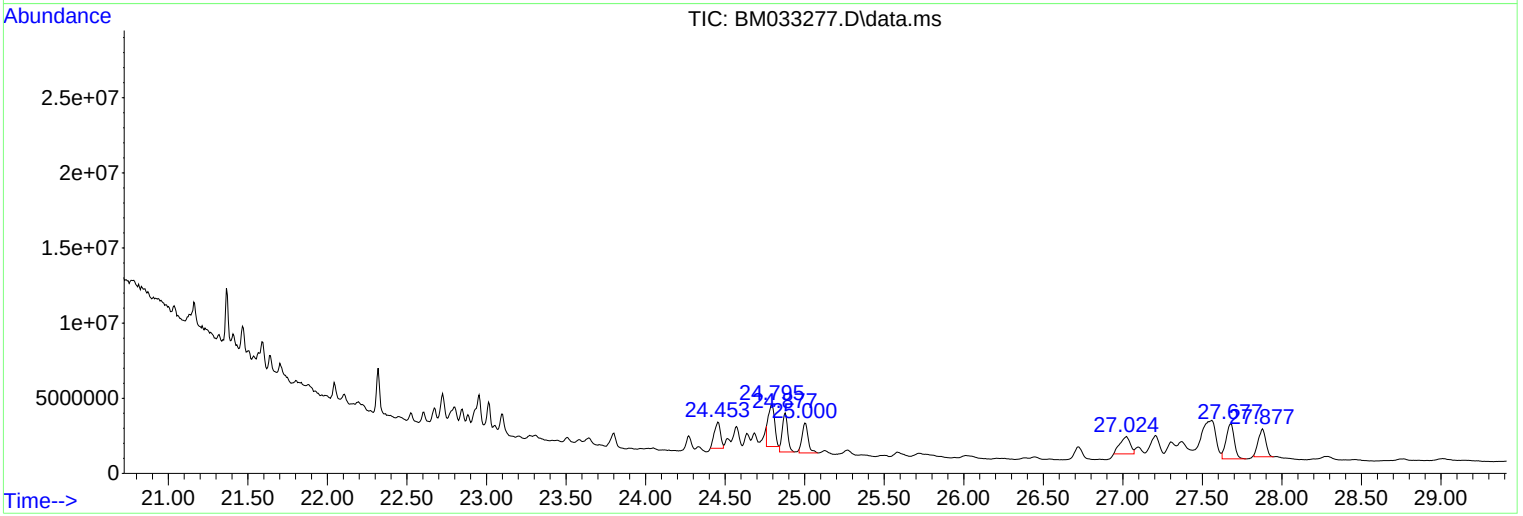
BNA_M
ClientSampleId :
261-262

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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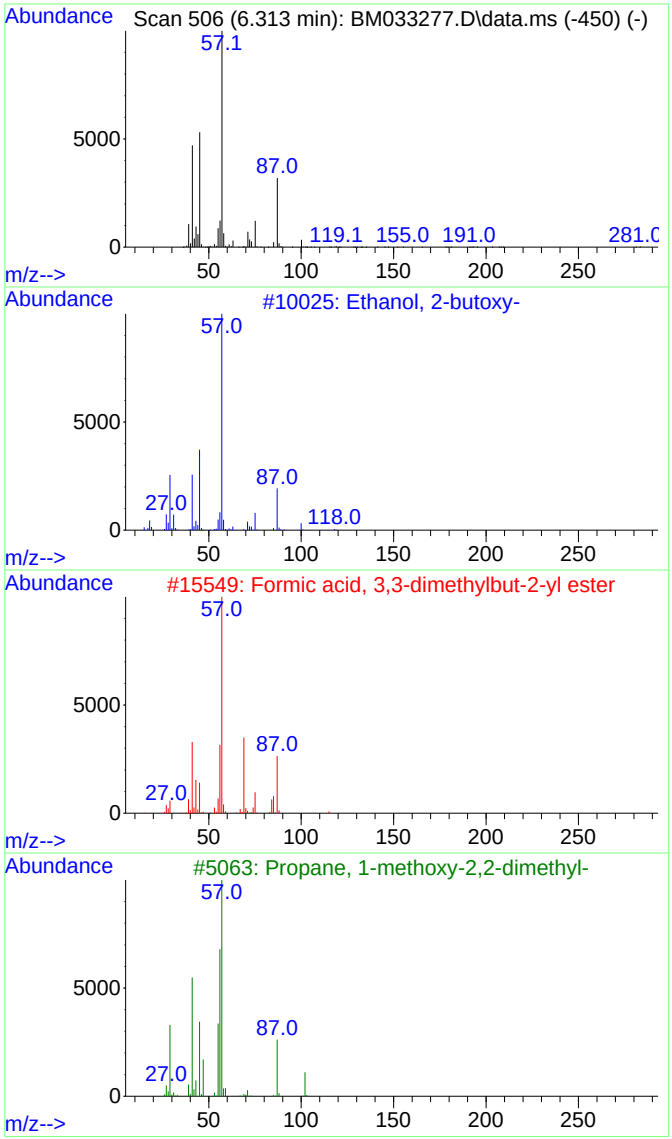
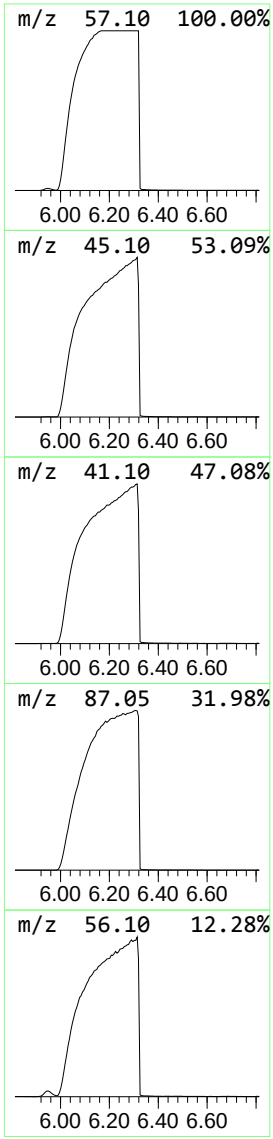
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.313	828.00 ng	432784000	1,4-Dichlorobenzene-d4	7.949

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	83
2	Formic acid, 3,3-dimethylbut-2-y...	130	C7H14O2	1000368-20-5	59
3	Propane, 1-methoxy-2,2-dimethyl-	102	C6H14O	001118-00-9	36
4	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	28
5	Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	27





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
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TIC Library : C:\Database\NIST20.L
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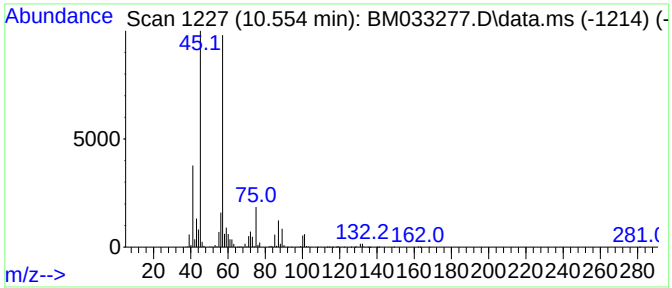
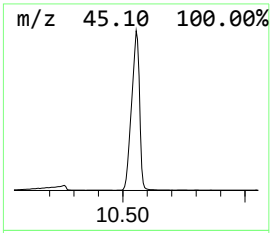
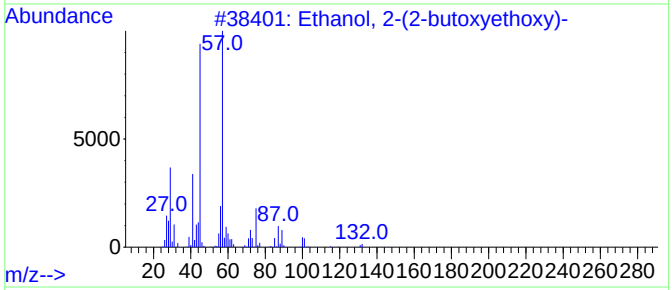
****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 11

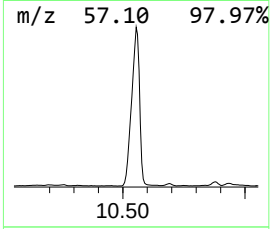
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.554	20.00 ng	9379630	Naphthalene-d8	10.737

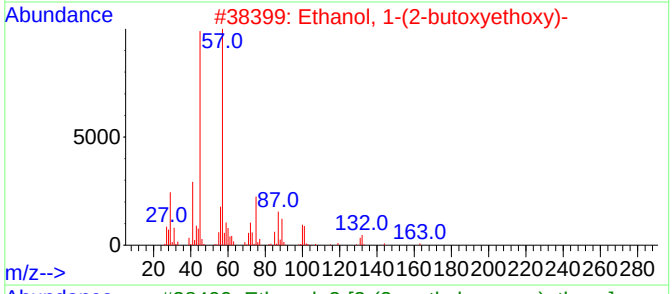
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
5	2-Heptanol, 3-methyl-	130	C8H18O	031367-46-1	50

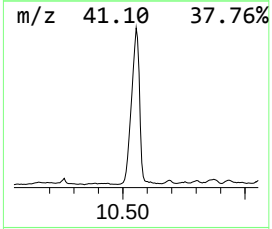


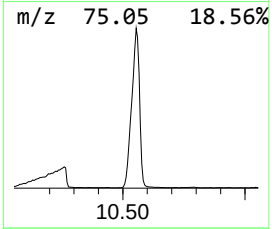


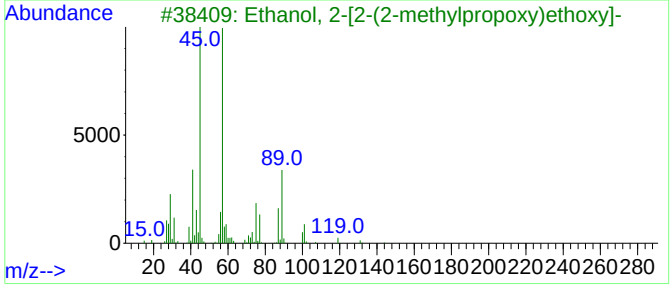


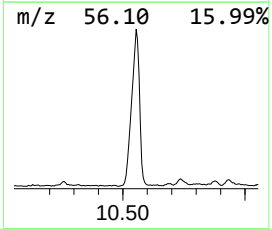












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Data File : BM033277.D
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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
261-262

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

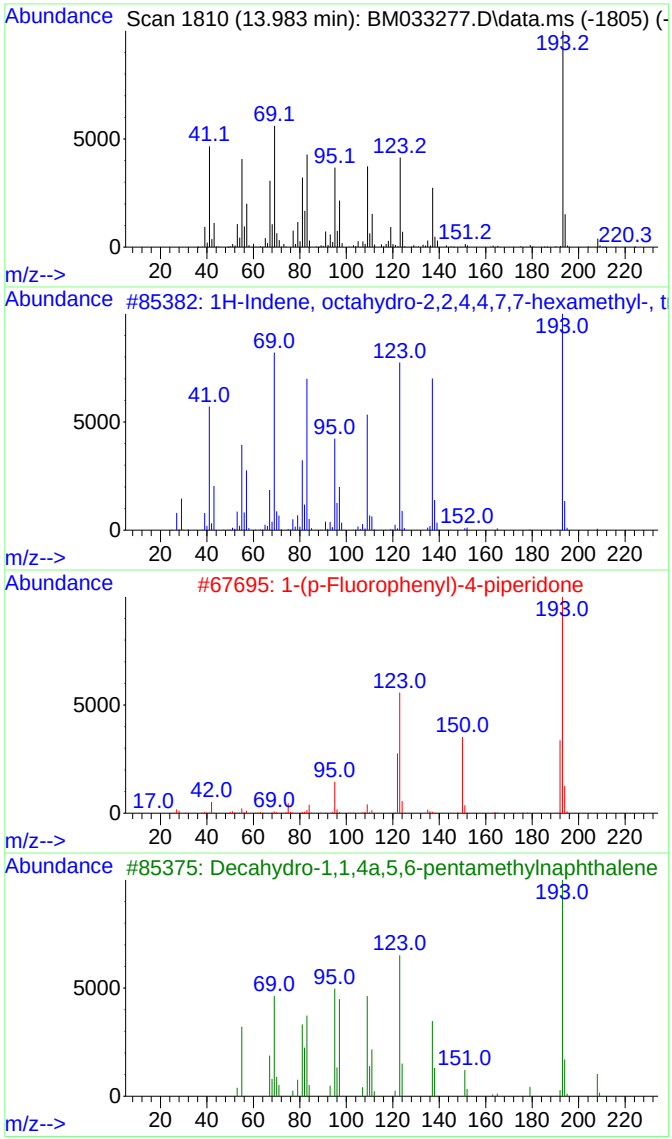
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

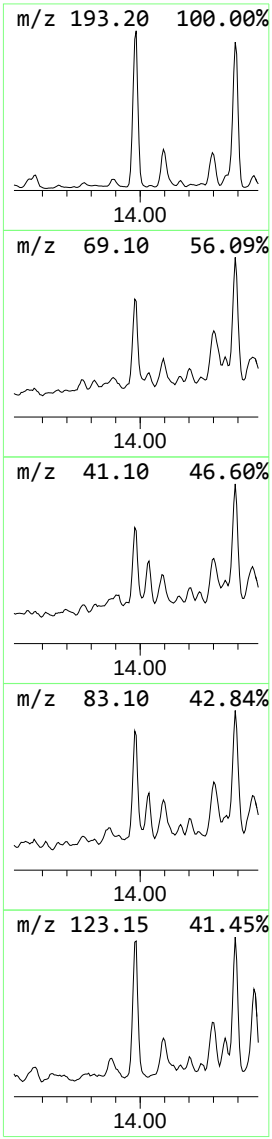
****

Peak Number 3 unknown13.983 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.983	23.66 ng	6437370	Acenaphthene-d10	14.560

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	40
2	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38
3	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	30
4	9-Phenanthrenamine	193	C14H11N	000947-73-9	27
5	Butan-2-one, 1-[3-(3,3-dimethyl-...	278	C16H26N2O2	1000303-34-2	27





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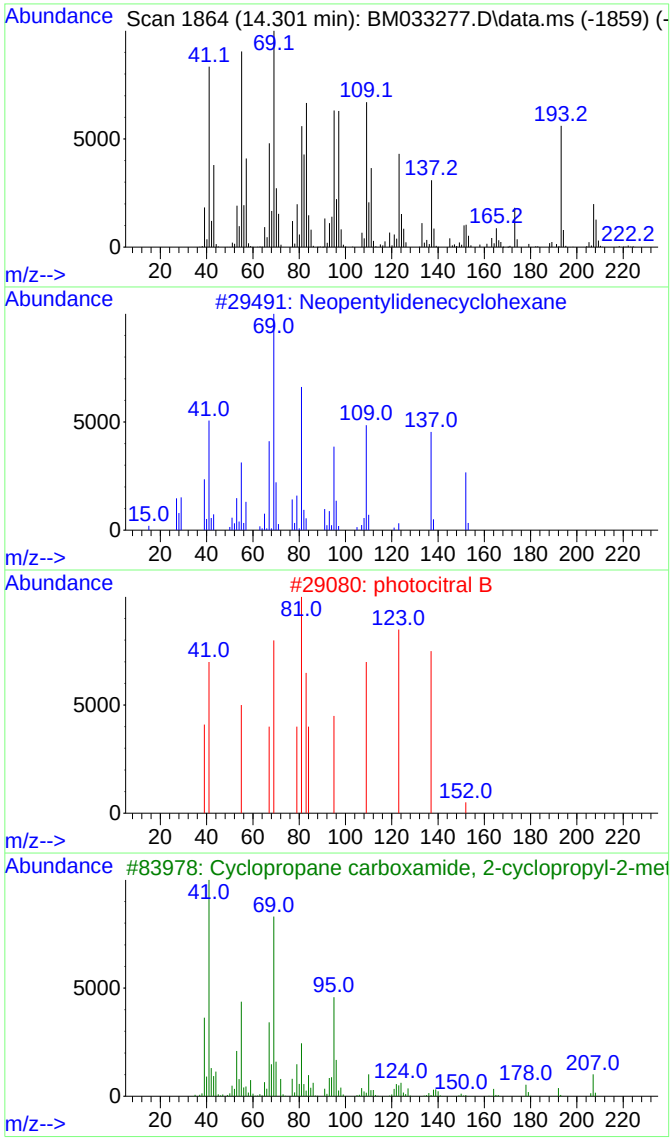
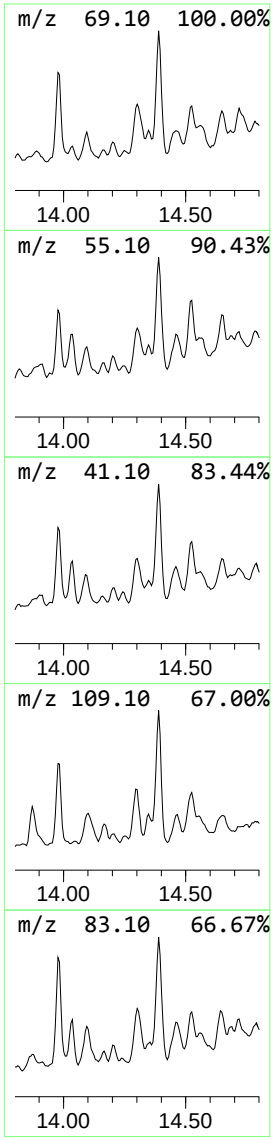
****

Peak Number 4 unknown14.301 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.301	18.78 ng	5109450	Acenaphthene-d10	14.560

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Neopentylidenecyclohexane	152	C11H20	039546-80-0	41
2	photocitral B	152	C10H16O	006040-45-5	38
3	Cyclopropane carboxamide, 2-cycl...	207	C13H21NO	331416-19-4	38
4	Citronellol	156	C10H20O	000106-22-9	27
5	(2,4,6-Trimethylcyclohexyl) meth...	156	C10H20O	013702-56-2	27





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Instrument :
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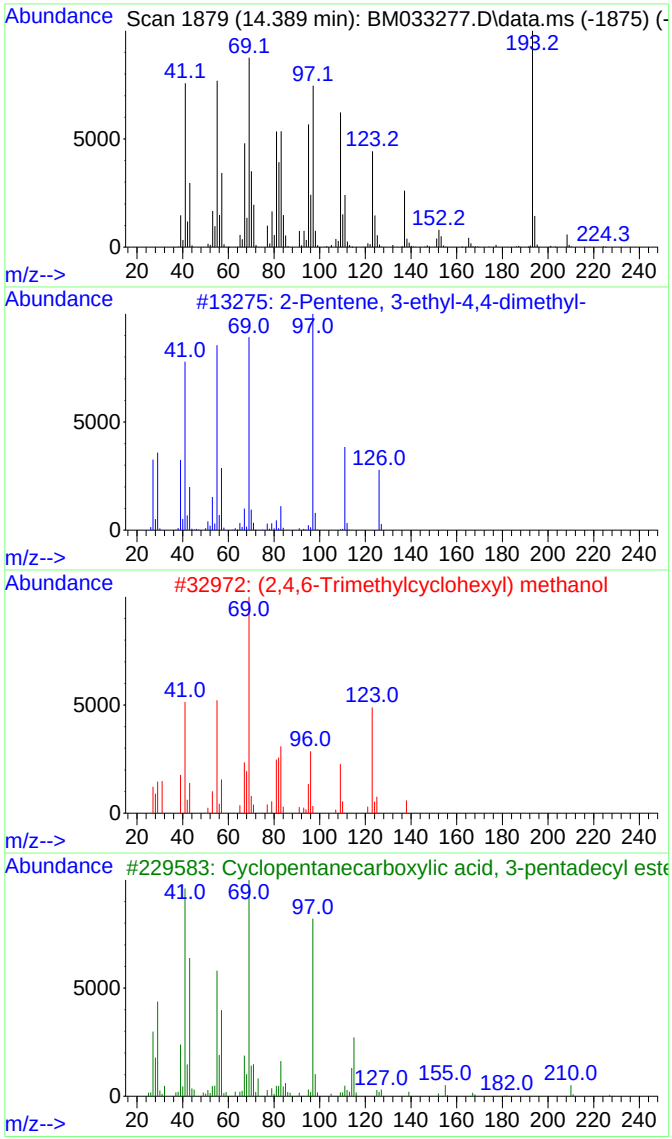
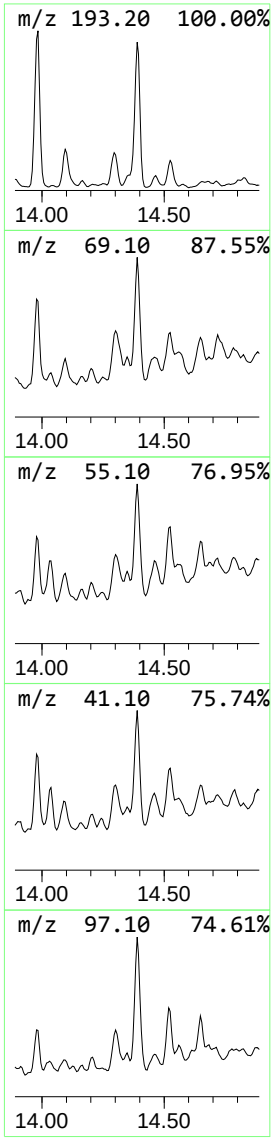
Peak Number 5 unknown14.389 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.389	34.62 ng	9419430	Acenaphthene-d10	14.560

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, 3-ethyl-4,4-dimethyl-	126	C9H18	053907-59-8	30
2	(2,4,6-Trimethylcyclohexyl) meth...	156	C10H20O	013702-56-2	22
3	Cyclopentanecarboxylic acid, 3-p...	324	C21H40O2	1000280-59-1	22
4	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	22
5	Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054823-96-0	18





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ClientSampleId :
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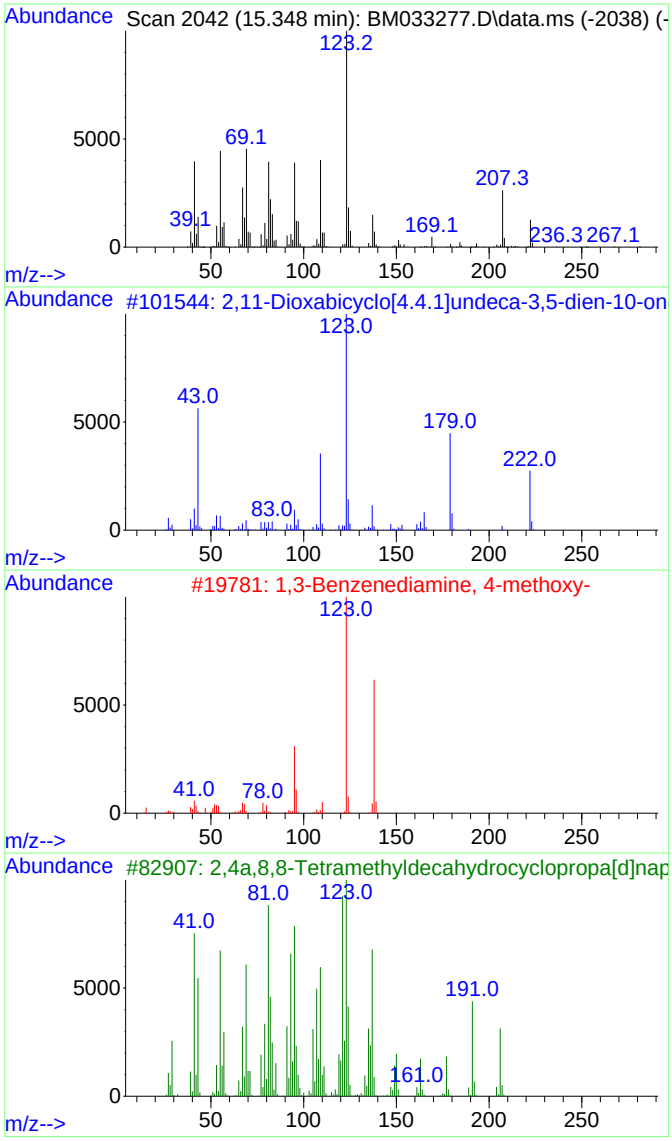
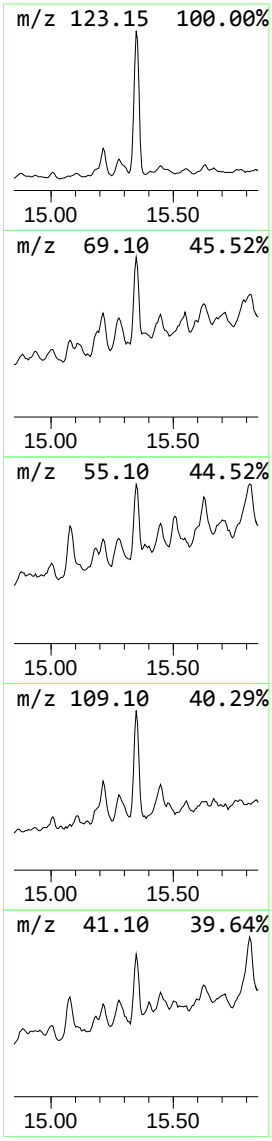
****
Peak Number 6 2,11-Dioxabicyclo[4.4.1]und... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.348	24.82 ng	6751600	Acenaphthene-d10	14.560

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,11-Dioxabicyclo[4.4.1]undeca-3...	222	C13H18O3	070412-52-1	53
2	1,3-Benzenediamine, 4-methoxy-	138	C7H10N2O	000615-05-4	47
3	2,4a,8,8-Tetramethyldecahydrocyc...	206	C15H26	074022-04-1	43
4	3-Fluorobenzoic acid, 2-ethylcyc...	250	C15H19FO2	1000279-04-9	43
5	1H-Pyrazole, 1,3,4,5-tetramethyl-	124	C7H12N2	001073-20-7	38





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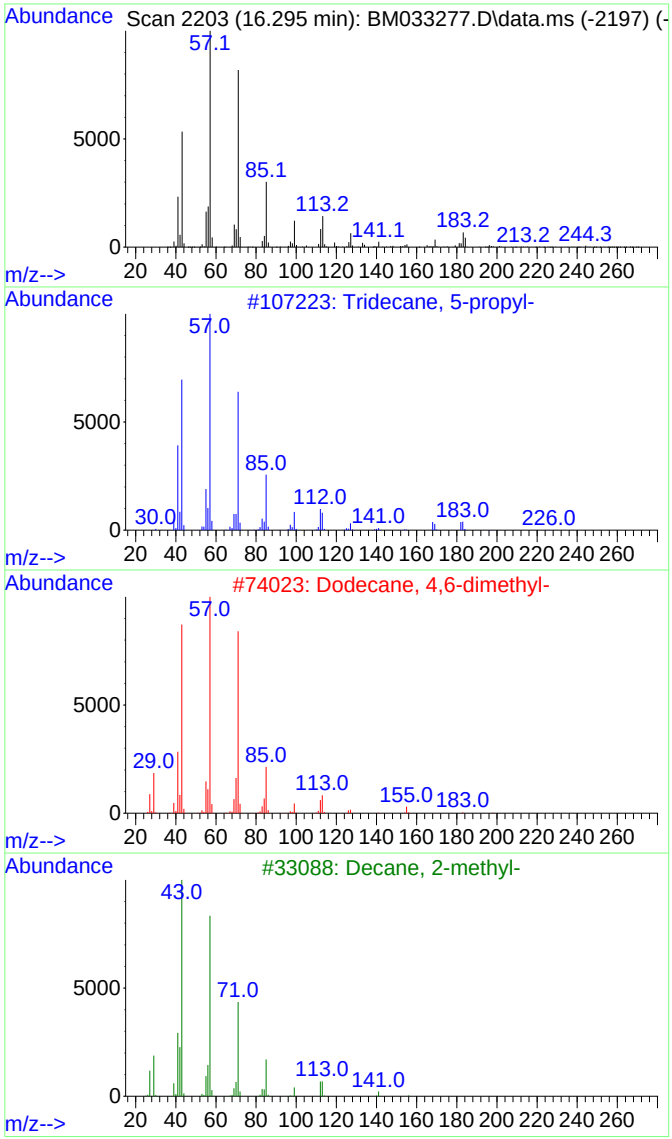
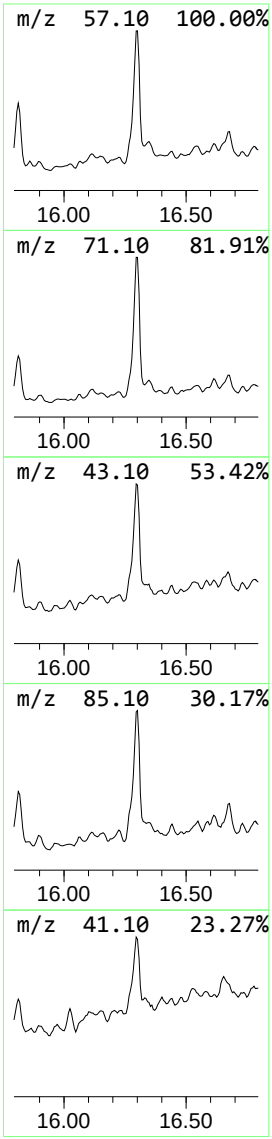
Peak Number 7 Tridecane, 5-propyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.295	20.00 ng	17870400	Phenanthrene-d10	17.313

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 5-propyl-	226	C16H34	055045-11-9	86
2	Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	83
3	Decane, 2-methyl-	156	C11H24	006975-98-0	80
4	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	72
5	Decane, 3,7-dimethyl-	170	C12H26	017312-54-8	68





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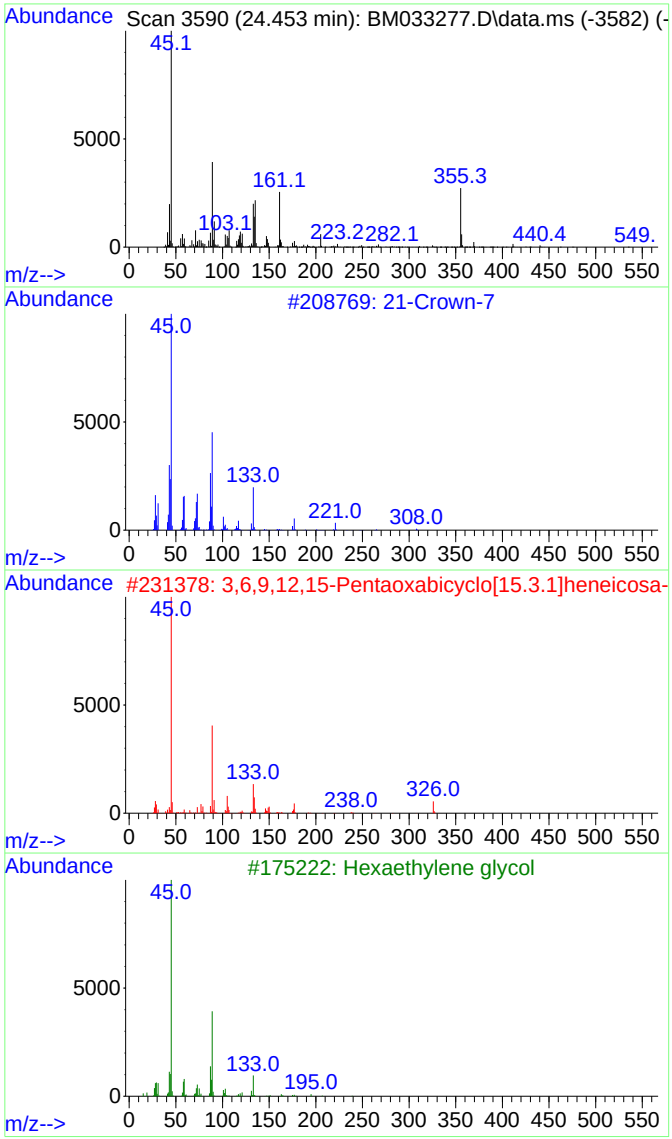
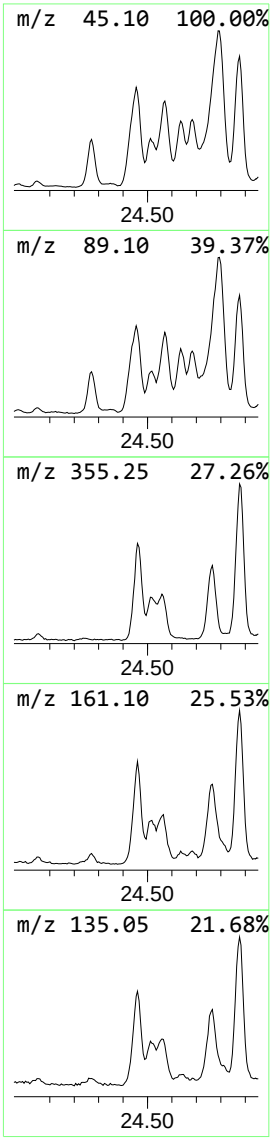
Peak Number 8 unknown24.453 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.453	20.00 ng	4772280	Perylene-d12	23.801

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	21-Crown-7	308	C14H28O7	033089-36-0	40
2	3,6,9,12,15-Pentaoxabicyclo[15.3...	326	C17H26O6	071128-99-9	40
3	Hexaethylene glycol	282	C12H26O7	002615-15-8	38
4	3,6,9,12,15,18,21-Heptaoxabicycl...	462	C20H31BrO7	111982-23-1	37
5	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112621\
Data File : BM033277.D
Acq On : 26 Nov 2021 22:28
Operator : CG/JU
Sample : M4803-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
261-262

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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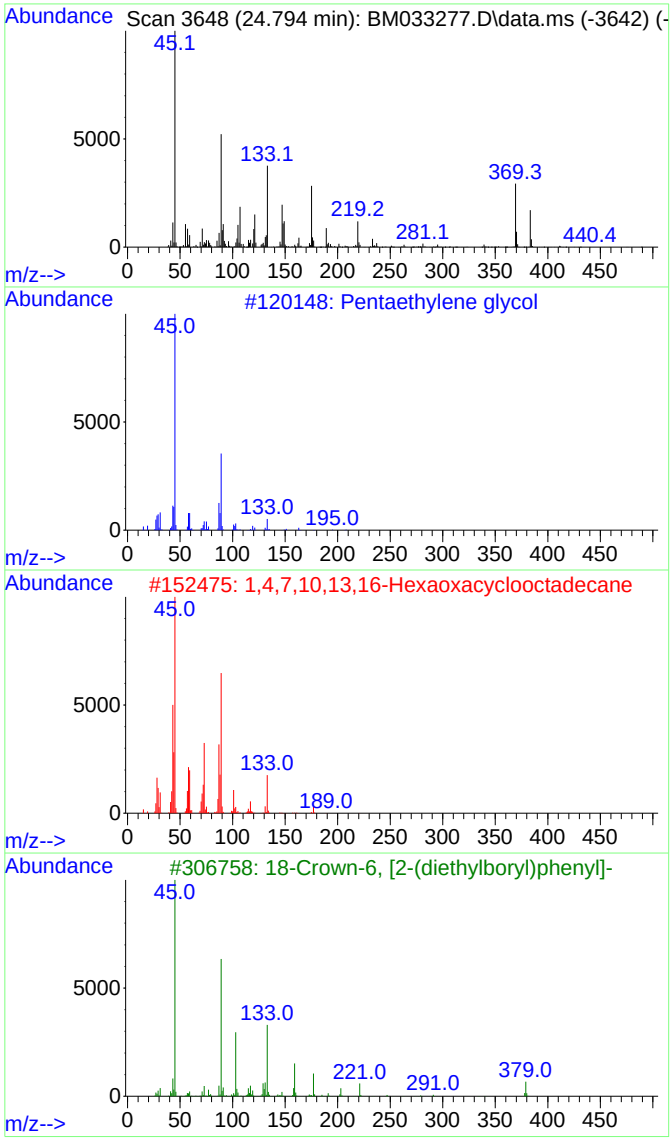
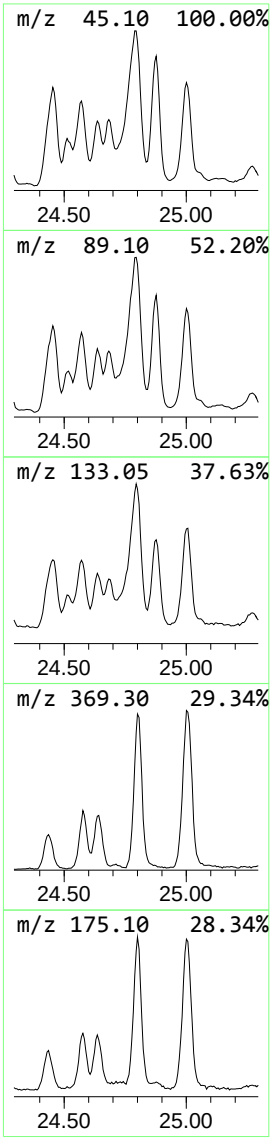
Peak Number 9 unknown24.794 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.794	32.06 ng	7650780	Perylene-d12	23.801

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentaethylene glycol	238	C10H22O6	004792-15-8	38
2	1,4,7,10,13,16-Hexaoxacyclooctad...	264	C12H24O6	017455-13-9	38
3	18-Crown-6, [2-(diethylboryl)phe...	408	C22H37BO6	1010161-99-8	38
4	15-Crown-5	220	C10H20O5	033100-27-5	38
5	3,6,9,12,15,18,21-Heptaoxabicycl...	462	C20H31BrO7	111982-23-1	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112621\
Data File : BM033277.D
Acq On : 26 Nov 2021 22:28
Operator : CG/JU
Sample : M4803-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
261-262

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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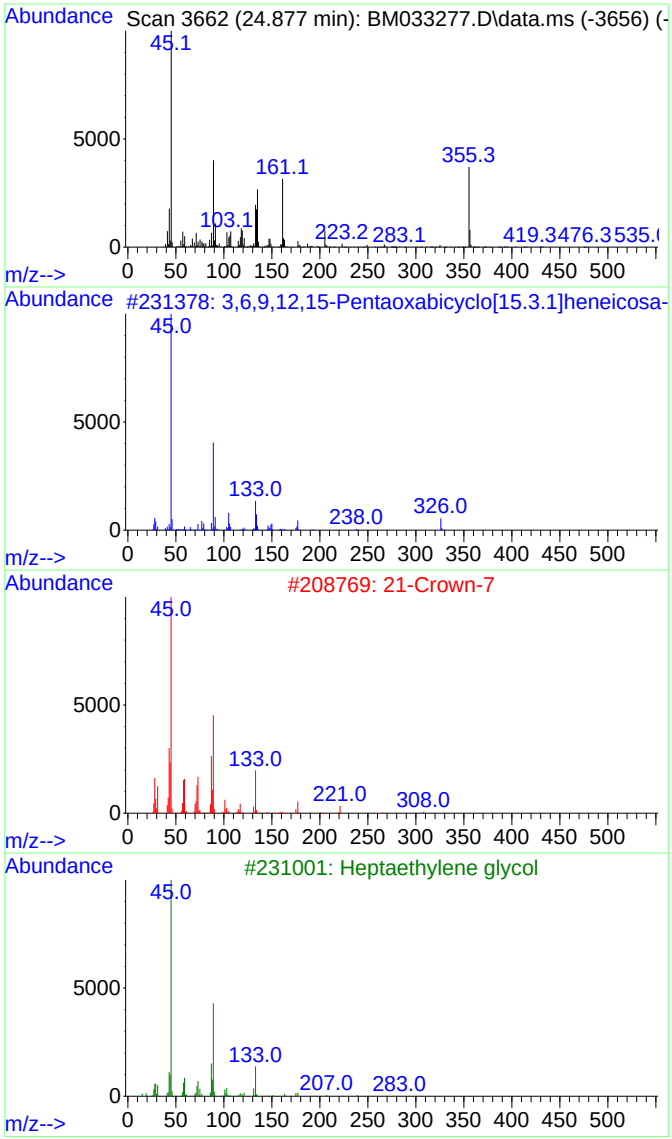
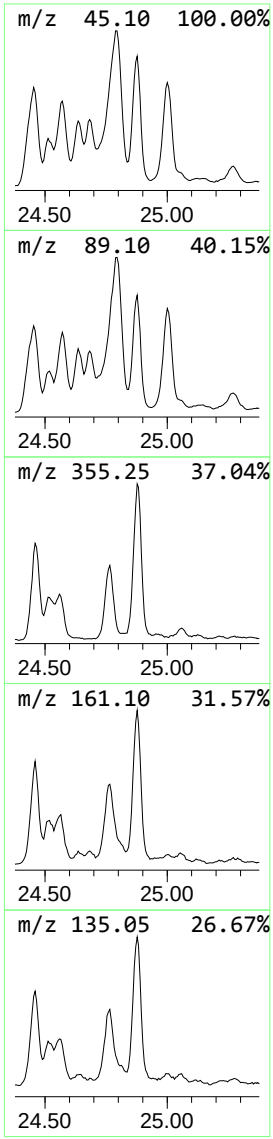
Peak Number 10 unknown24.877 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.877	25.14 ng	5998870	Perylene-d12	23.801

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6,9,12,15-Pentaoxabicyclo[15.3...	326	C17H26O6	071128-99-9	40
2	21-Crown-7	308	C14H28O7	033089-36-0	33
3	Heptaethylene glycol	326	C14H30O8	005617-32-3	28
4	1,4,7,10,13,16-Hexaoxanonadecane...	318	C16H30O6	1000163-64-0	28
5	15-Crown-5	220	C10H20O5	033100-27-5	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112621\
Data File : BM033277.D
Acq On : 26 Nov 2021 22:28
Operator : CG/JU
Sample : M4803-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
261-262

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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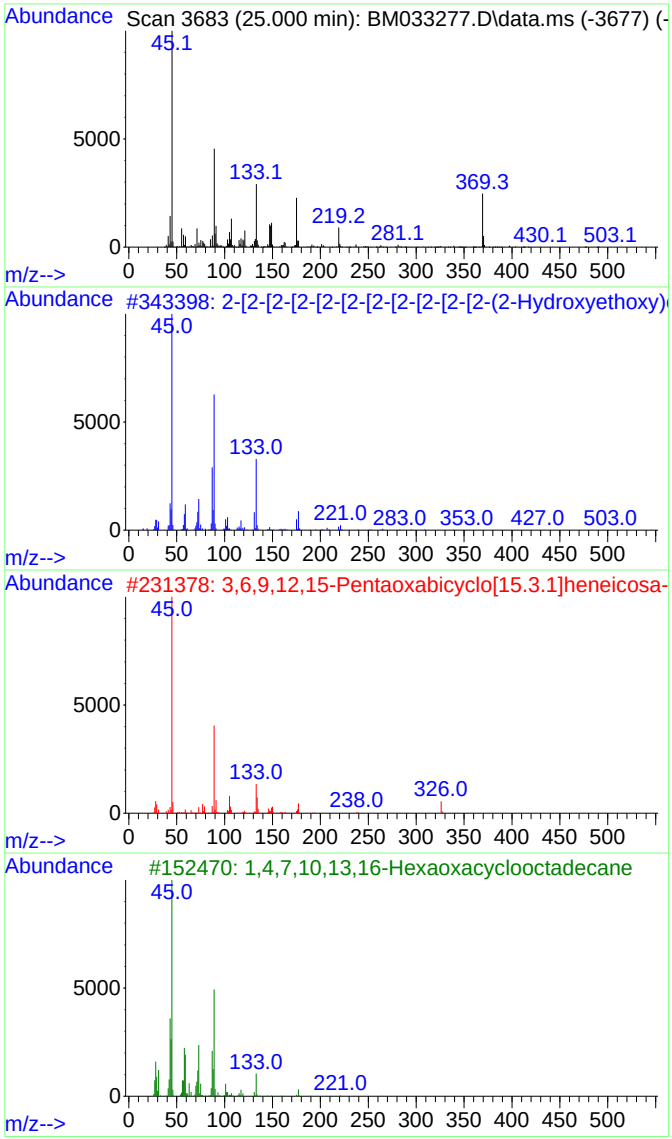
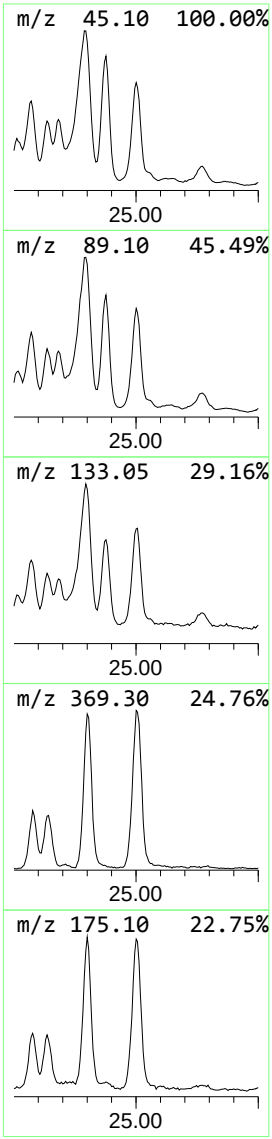
Peak Number 11 unknown25.000 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.000	21.86 ng	5216490	Perylene-d12	23.801

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-[2-[2-[2-[2-...	546	C24H50O13	1000352-12-7	42
2	3,6,9,12,15-Pentaoxabicyclo[15.3...	326	C17H26O6	071128-99-9	38
3	1,4,7,10,13,16-Hexaoxacyclooctad...	264	C12H24O6	017455-13-9	37
4	18-Crown-6, [2-(diethylboryl)phe...	408	C22H37BO6	1010161-99-8	28
5	Pentaethylene glycol	238	C10H22O6	004792-15-8	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112621\
Data File : BM033277.D
Acq On : 26 Nov 2021 22:28
Operator : CG/JU
Sample : M4803-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
261-262

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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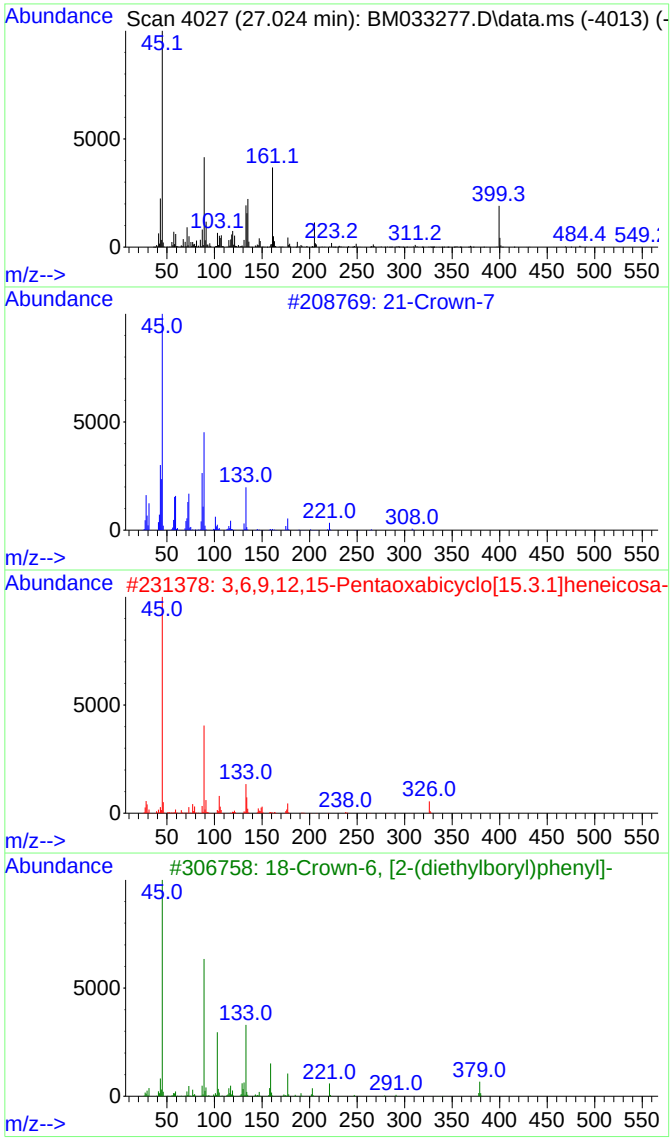
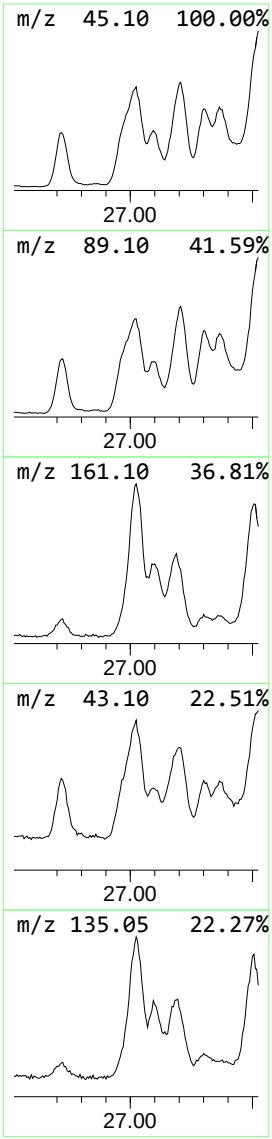
Peak Number 12 unknown27.024 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.024	22.03 ng	5255500	Perylene-d12	23.801

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	21-Crown-7	308	C14H28O7	033089-36-0	47
2	3,6,9,12,15-Pentaoxabicyclo[15.3...	326	C17H26O6	071128-99-9	40
3	18-Crown-6, [2-(diethylboryl)phe...	408	C22H37BO6	1010161-99-8	38
4	3,6,9,12,15,18,21-Heptaoxabicycl...	462	C20H31BrO7	111982-23-1	37
5	Heptaethylene glycol	326	C14H30O8	005617-32-3	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112621\
Data File : BM033277.D
Acq On : 26 Nov 2021 22:28
Operator : CG/JU
Sample : M4803-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
261-262

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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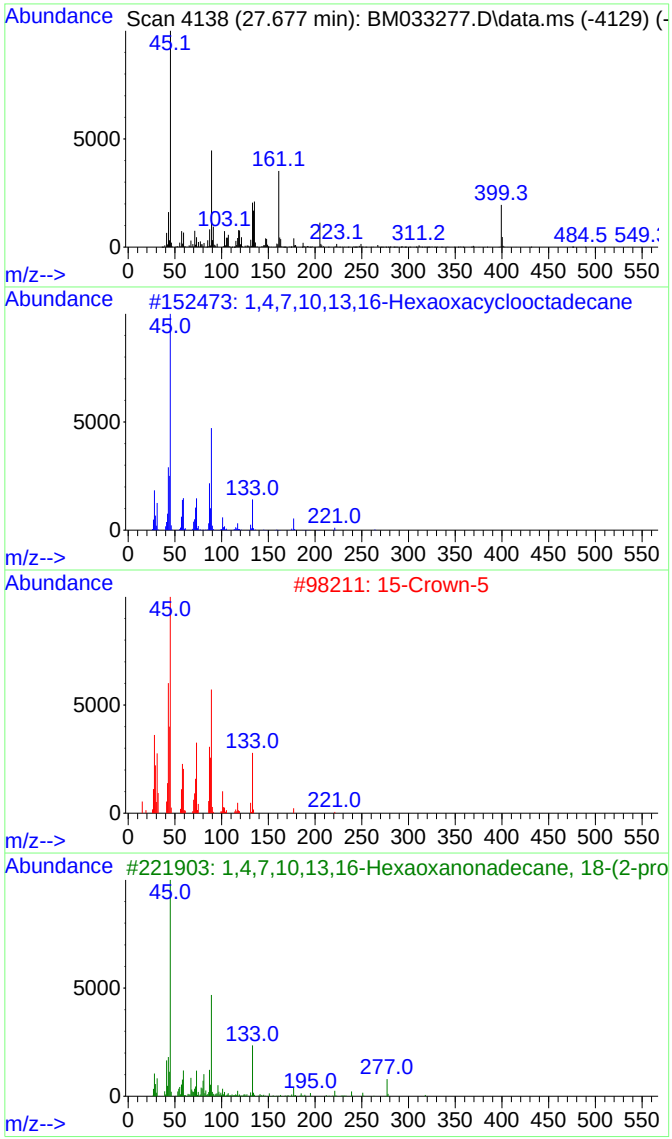
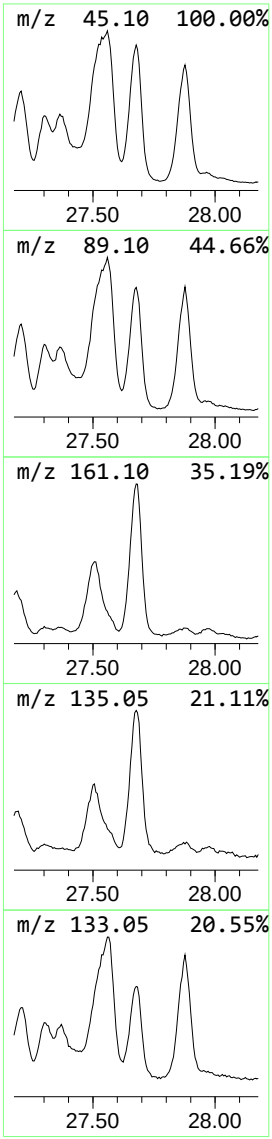
Peak Number 13 unknown27.677 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.677	34.36 ng	8198390	Perylene-d12	23.801

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4,7,10,13,16-Hexaoxacyclooctad...	264	C12H24O6	017455-13-9	38
2	15-Crown-5	220	C10H20O5	033100-27-5	38
3	1,4,7,10,13,16-Hexaoxanonadecane...	318	C16H30O6	1000163-64-0	38
4	3,6,9,12,15,18,21-Heptaoxabicycl...	462	C20H31BrO7	111982-23-1	37
5	3,6,9,12,15-Pentaoxabicyclo[15.3...	326	C17H26O6	071128-99-9	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112621\
Data File : BM033277.D
Acq On : 26 Nov 2021 22:28
Operator : CG/JU
Sample : M4803-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
261-262

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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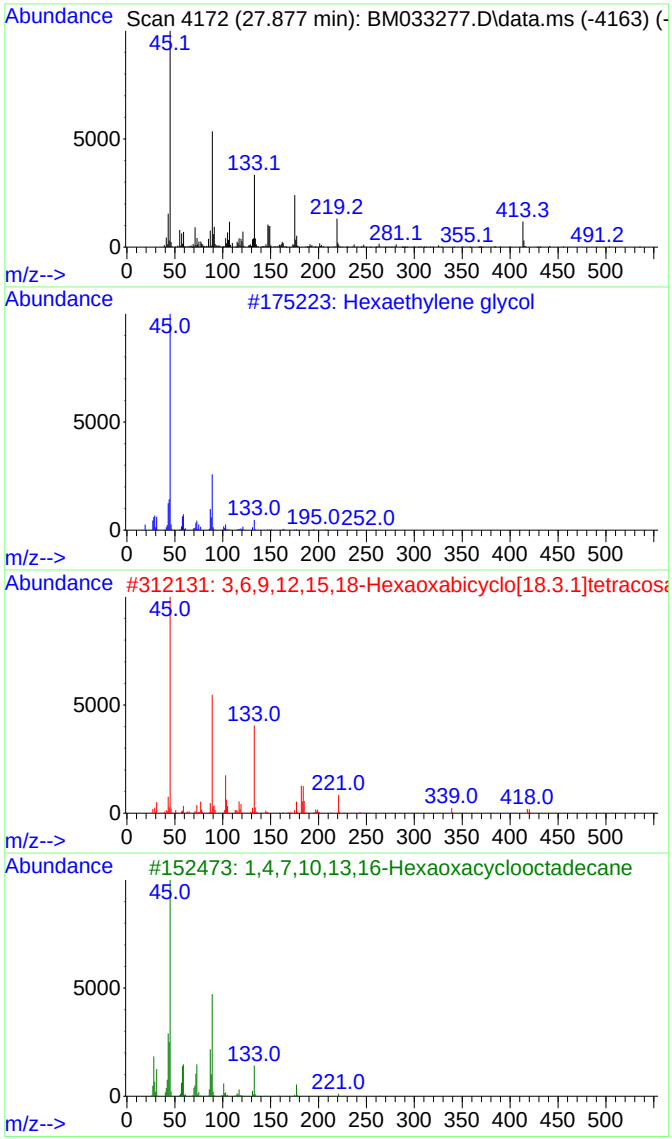
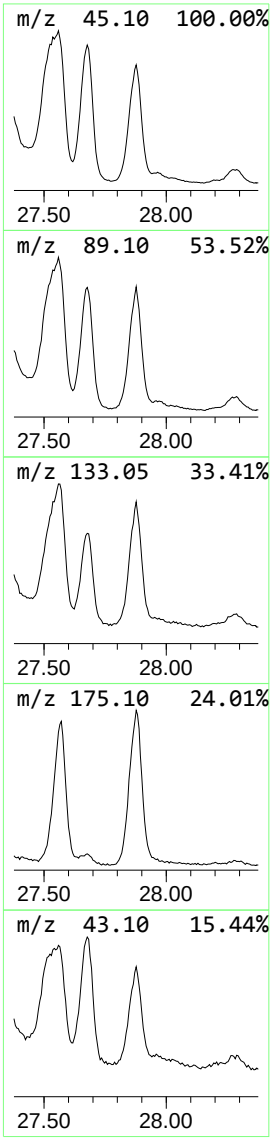
Peak Number 14 Hexaethylene glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.877	25.21 ng	6015090	Perylene-d12	23.801

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexaethylene glycol	282	C12H26O7	002615-15-8	50
2	3,6,9,12,15,18-Hexaoxabicyclo[18...	418	C18H27BrO6	111982-22-0	50
3	1,4,7,10,13,16-Hexaoxacyclooctad...	264	C12H24O6	017455-13-9	47
4	Nonaethylene glycol, TBDMS deriv...	528	C24H52O10Si	1010352-11-3	42
5	3,6,9,12,15,18,21-Heptaoxabicycl...	462	C20H31BrO7	111982-23-1	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112621\
Data File : BM033277.D
Acq On : 26 Nov 2021 22:28
Operator : CG/JU
Sample : M4803-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
261-262

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethanol, 2-butoxy-	6.313	828.0	ng	432784000	1	7.949	10453700	20.0
Ethanol, 2-(2-b...	10.554	20.0	ng	9379630	2	10.737	9379630	20.0
unknown13.983	13.983	23.7	ng	6437370	3	14.560	5441300	20.0
unknown14.301	14.301	18.8	ng	5109450	3	14.560	5441300	20.0
unknown14.389	14.389	34.6	ng	9419430	3	14.560	5441300	20.0
2,11-Dioxabicyc...	15.348	24.8	ng	6751600	3	14.560	5441300	20.0
Tridecane, 5-pr...	16.295	20.0	ng	17870400	4	17.313	17870400	20.0
unknown24.453	24.453	20.0	ng	4772280	6	23.801	4772280	20.0
unknown24.794	24.794	32.1	ng	7650780	6	23.801	4772280	20.0
unknown24.877	24.877	25.1	ng	5998870	6	23.801	4772280	20.0
unknown25.000	25.000	21.9	ng	5216490	6	23.801	4772280	20.0
unknown27.024	27.024	22.0	ng	5255500	6	23.801	4772280	20.0
unknown27.677	27.677	34.4	ng	8198390	6	23.801	4772280	20.0
Hexaethylene gl...	27.877	25.2	ng	6015090	6	23.801	4772280	20.0