

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080723\
 Data File : BM041310.D
 Acq On : 07 Aug 2023 13:43
 Operator : MA/JU
 Sample : 03903-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 MW-03

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-BM072823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM041310.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.899	283	291	298	rBV	44571	73342	1.34%	0.230%
2	5.363	363	370	384	rBV	1562137	2338320	42.69%	7.321%
3	6.969	636	643	660	rBV	1584344	2534467	46.27%	7.935%
4	7.787	772	782	793	rBV	449327	703012	12.83%	2.201%
5	8.963	974	982	998	rBV	920172	1562052	28.51%	4.891%
6	10.592	1252	1259	1280	rBV	585197	1021681	18.65%	3.199%
7	13.069	1674	1680	1695	rBV	2345203	3498057	63.86%	10.952%
8	14.457	1907	1916	1926	rBV	1037473	1489162	27.18%	4.662%
9	15.133	2009	2031	2033	rBV2	100703	537467	9.81%	1.683%
10	15.827	2144	2149	2158	rBV	166558	226078	4.13%	0.708%
11	15.957	2165	2171	2187	rBV	2431115	3398080	62.03%	10.639%
12	17.215	2379	2385	2392	rBV	1464608	1964166	35.86%	6.149%
13	17.339	2402	2406	2410	rVB3	45437	60814	1.11%	0.190%
14	18.115	2533	2538	2550	rBV	1192106	1795508	32.78%	5.621%
15	19.398	2752	2756	2778	rVB	543938	817214	14.92%	2.559%
16	19.851	2828	2833	2843	rBV	4344636	5478047	100.00%	17.151%
17	21.127	3046	3050	3060	rBV	292657	440130	8.03%	1.378%
18	21.421	3095	3100	3111	rBV	1775621	2115274	38.61%	6.623%
19	23.792	3497	3503	3513	rVB	972685	1887619	34.46%	5.910%

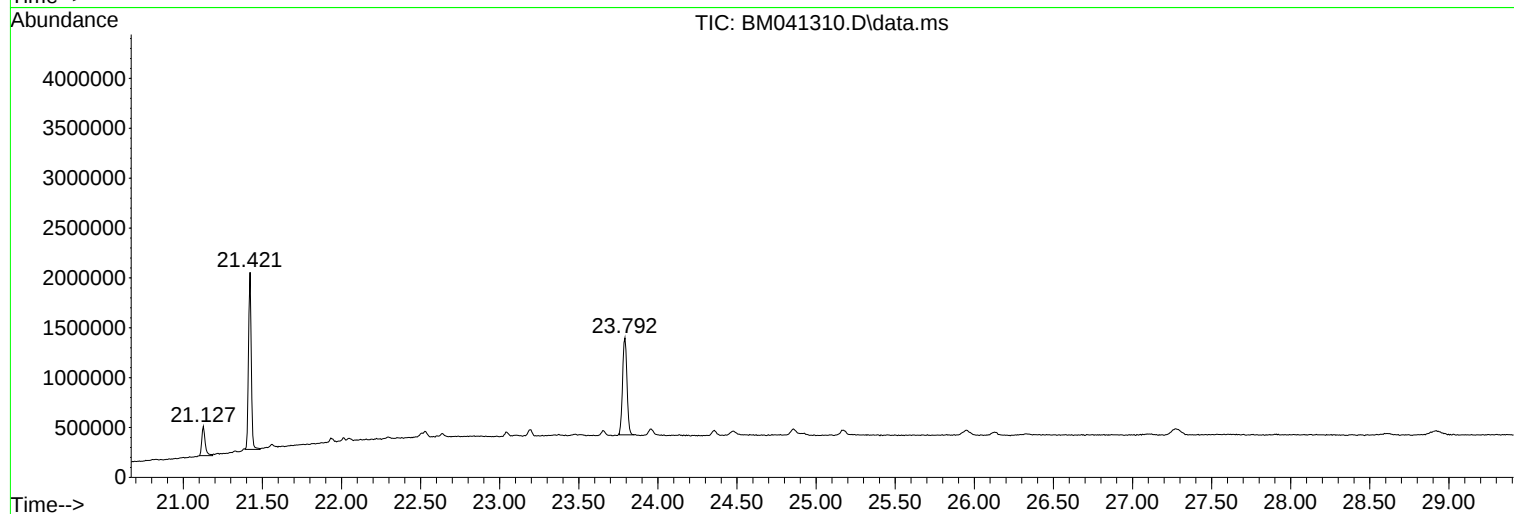
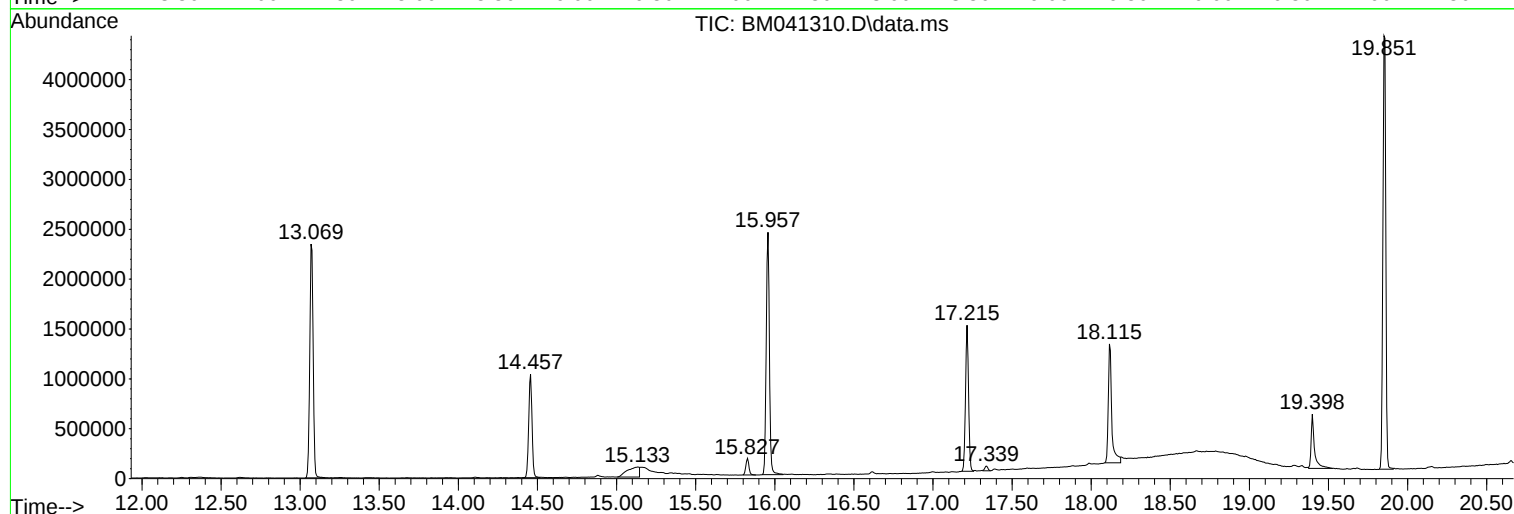
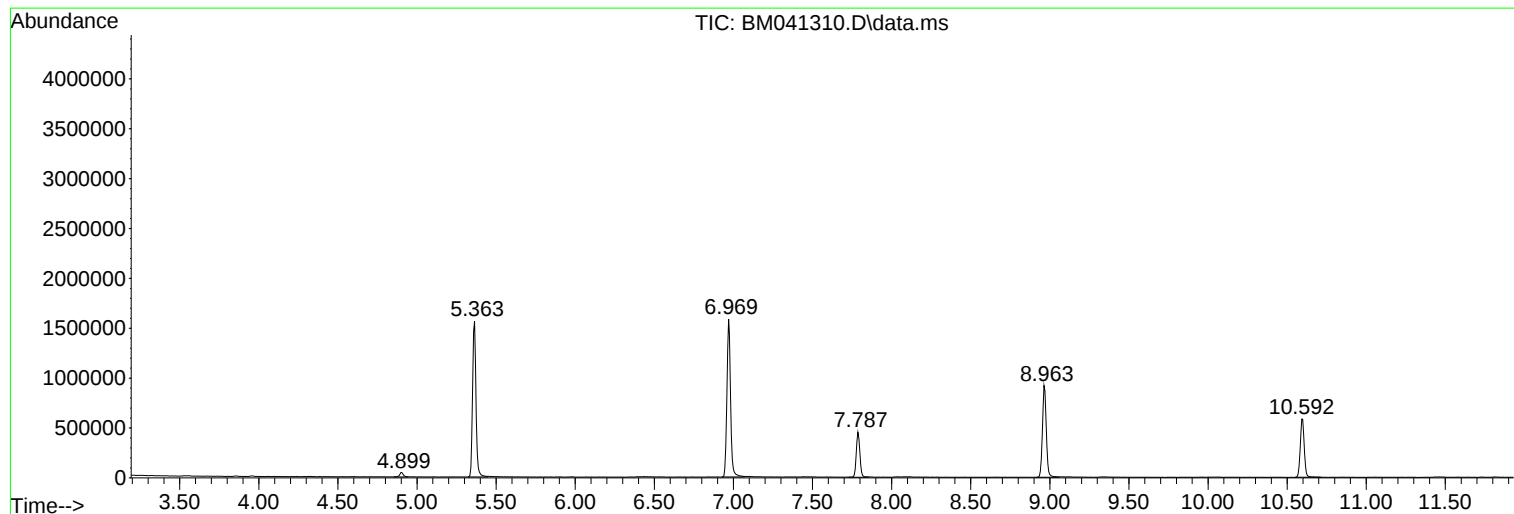
Sum of corrected areas: 31940490

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.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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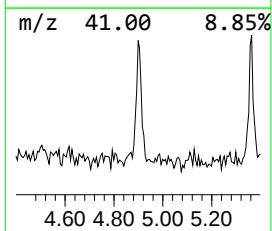
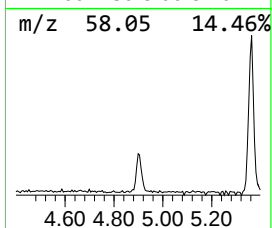
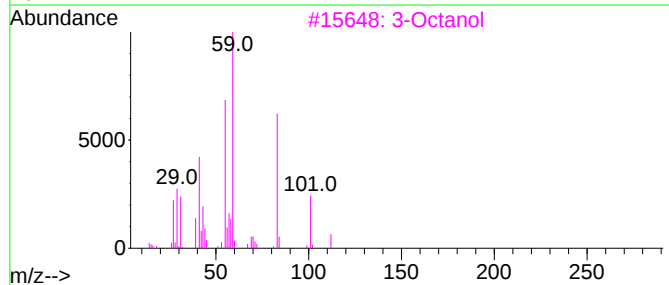
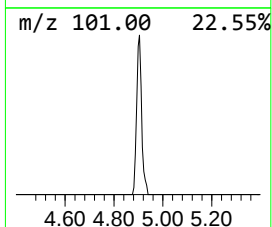
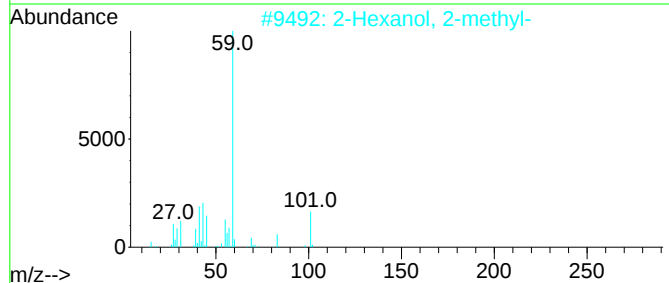
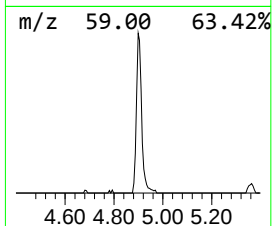
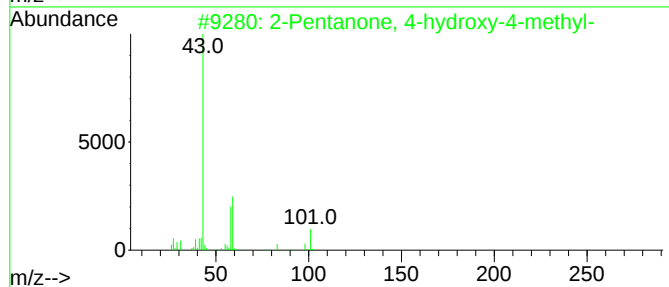
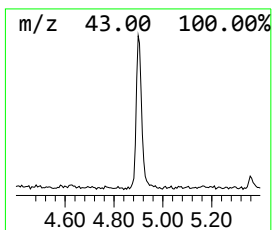
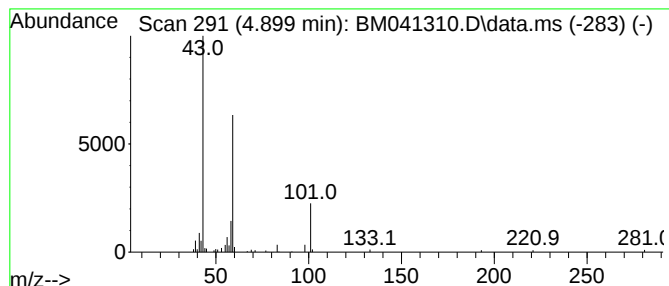
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.899	2.09 ng	73342	1,4-Dichlorobenzene-d4	7.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	42		
3	3-Octanol	130	C8H18O	000589-98-0	38		
4	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33		
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25		



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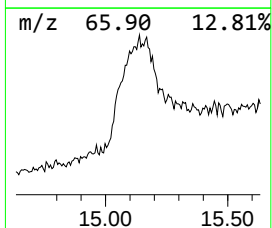
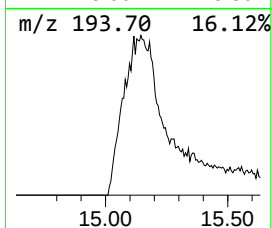
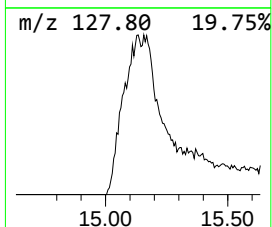
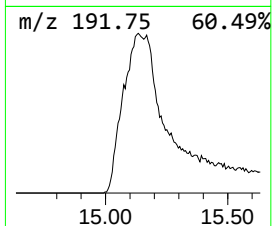
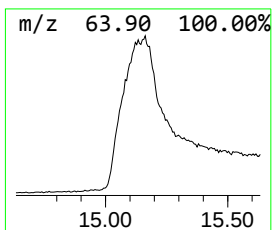
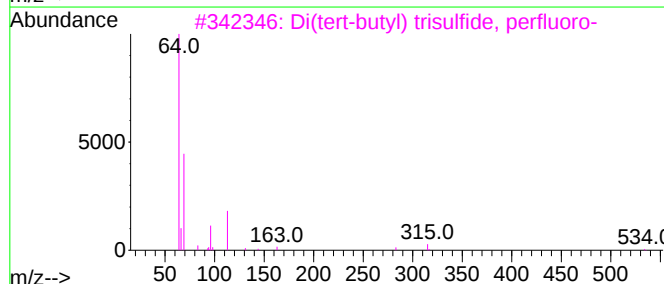
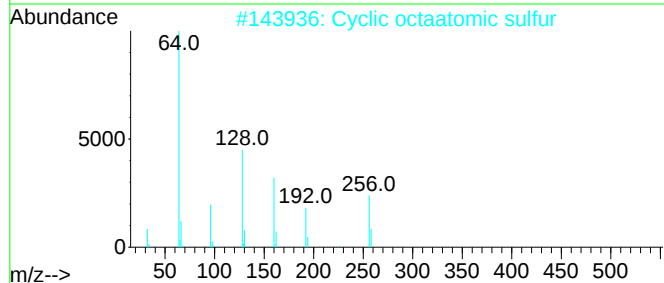
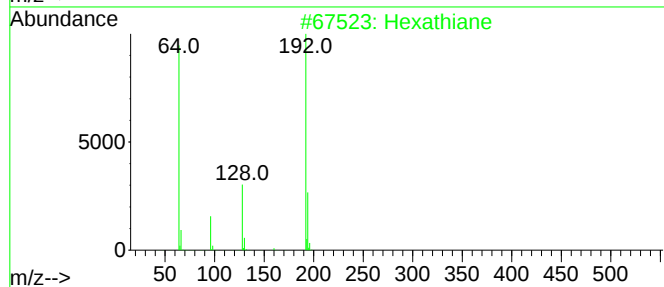
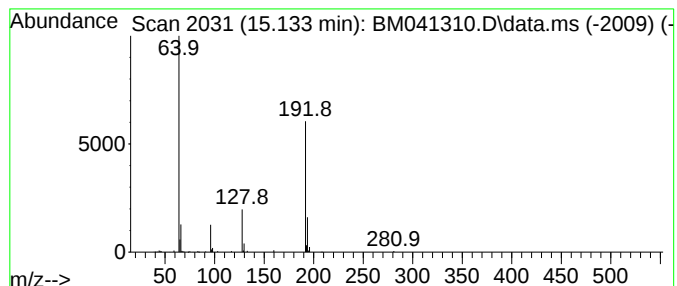
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Hexathiane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.133	7.22 ng	537467	Acenaphthene-d10	14.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexathiane	192	S6	013798-23-7	94
2			Cyclic octaatomic sulfur	256	S8	010544-50-0	9
3			Di(tert-butyl) trisulfide, perfl...	534	C8F18S3	016005-64-4	9
4			2-Chloro-7-methoxynaphthalene	192	C11H9ClO	067061-67-0	5
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	4



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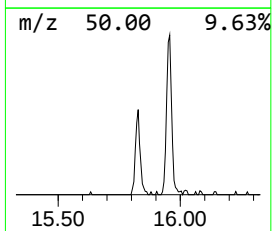
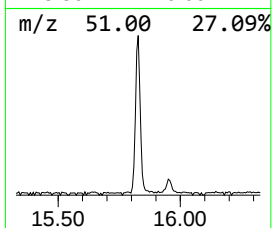
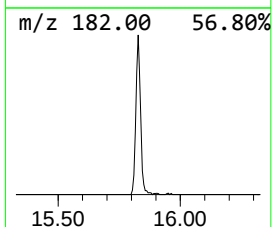
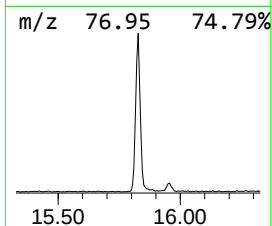
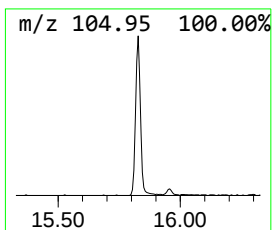
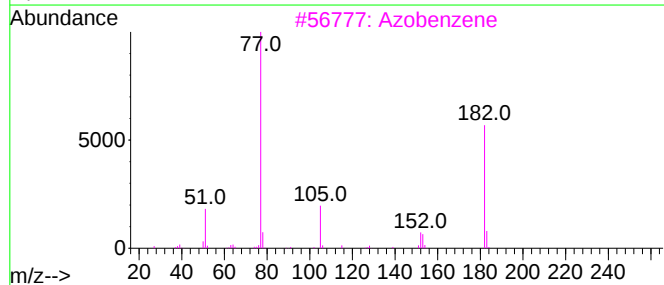
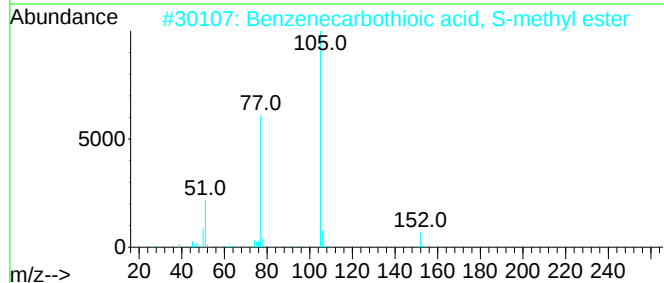
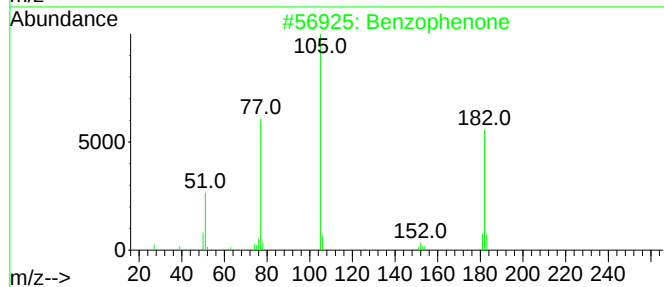
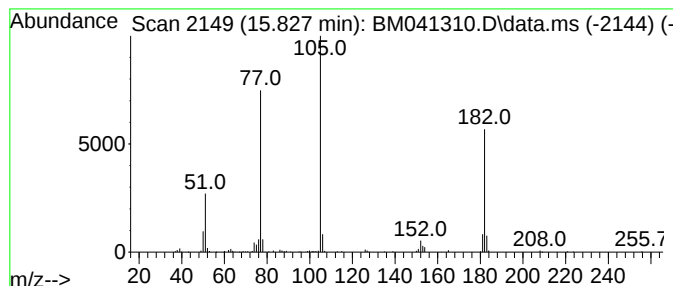
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Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.827	3.04 ng	226078	Acenaphthene-d10	14.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	68
3			Azobenzene	182	C12H10N2	000103-33-3	64
4			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	53
5			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	53



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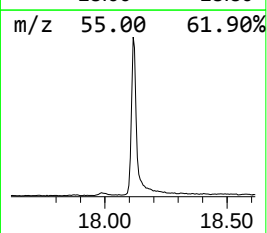
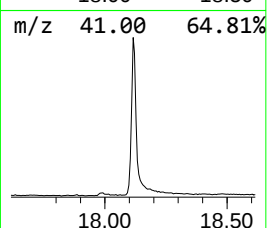
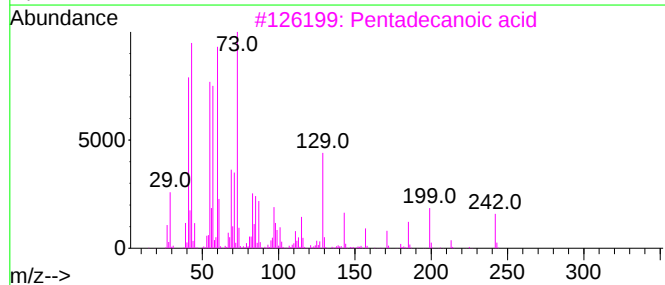
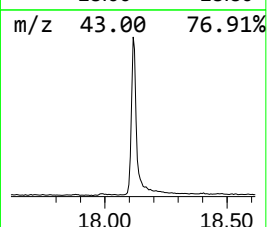
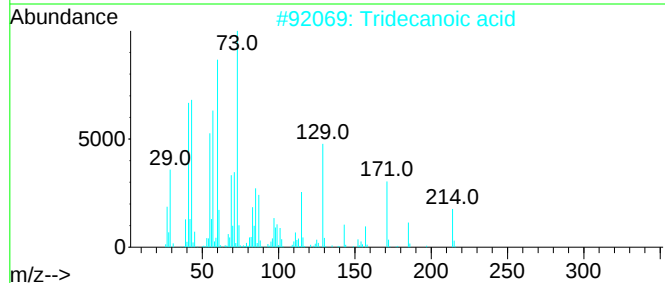
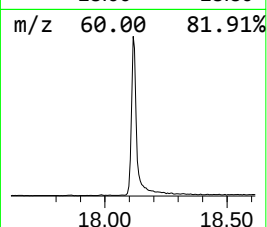
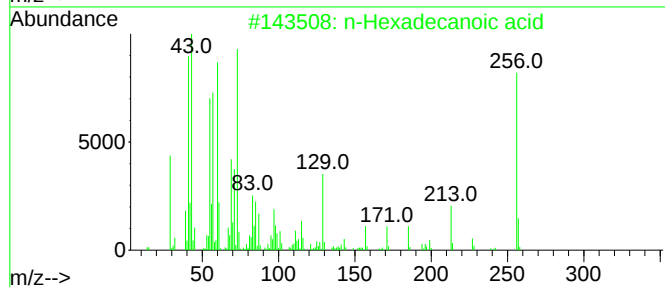
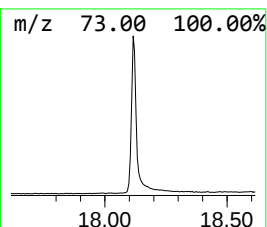
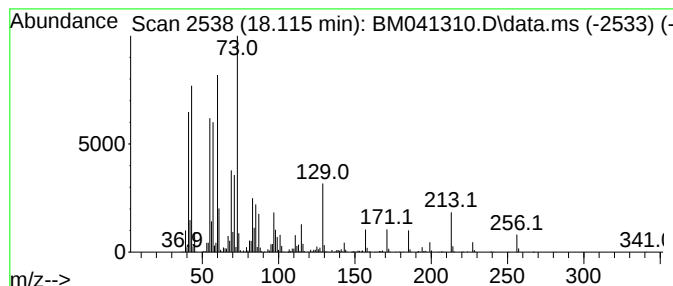
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.115	18.28 ng	1795510	Phenanthrene-d10	17.215

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5			Nonanoic acid	158	C9H18O2	000112-05-0	58



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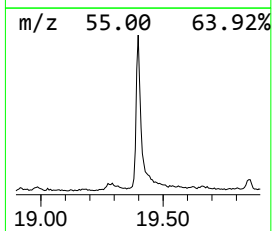
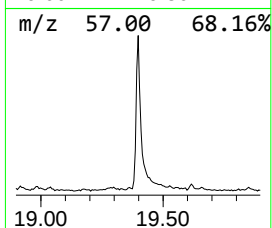
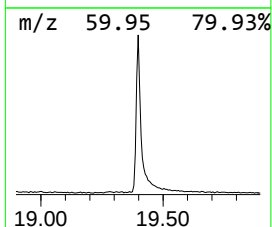
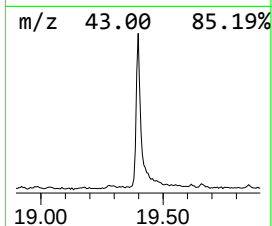
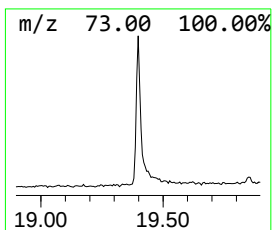
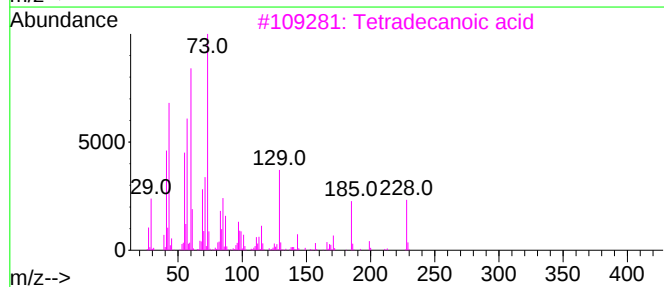
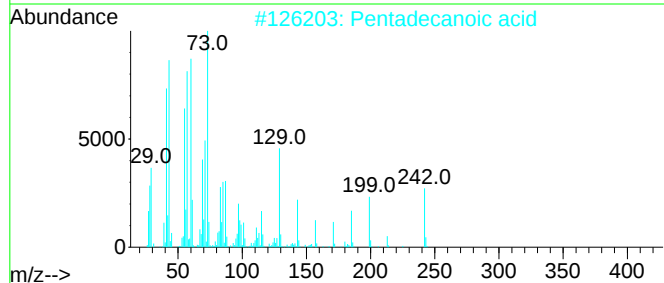
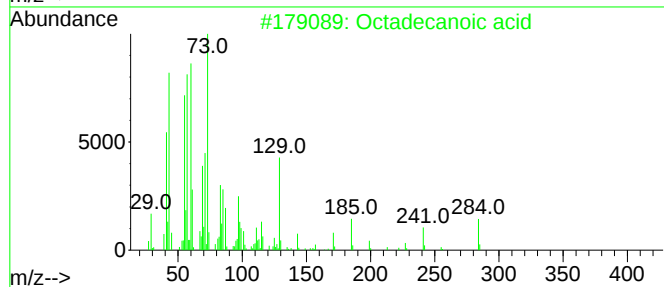
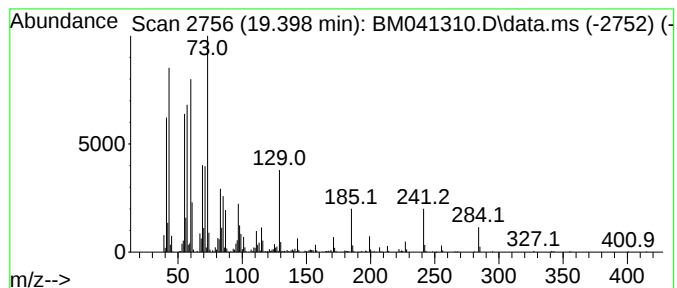
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Peak Number 5 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.398	7.73 ng	817214	Chrysene-d12	21.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	70
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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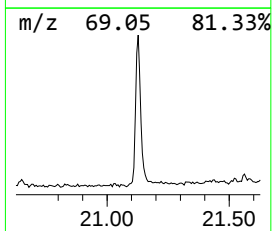
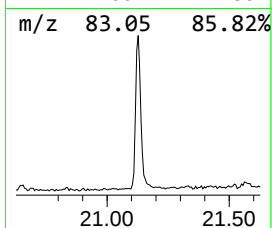
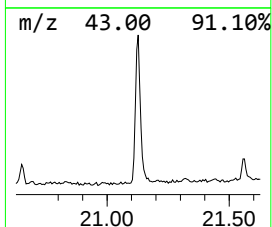
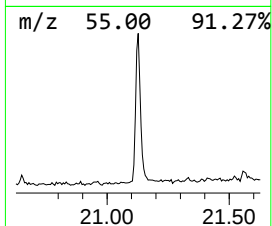
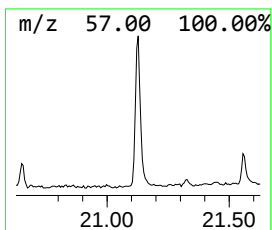
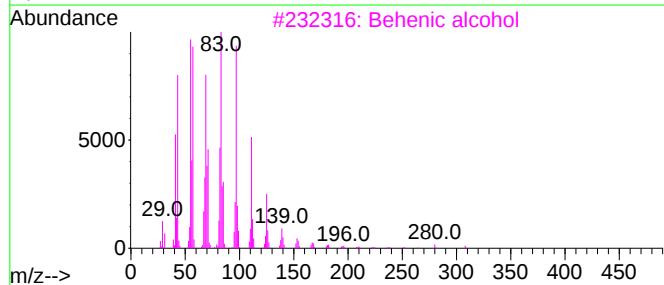
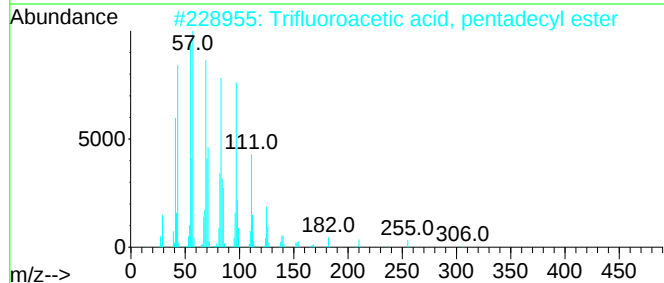
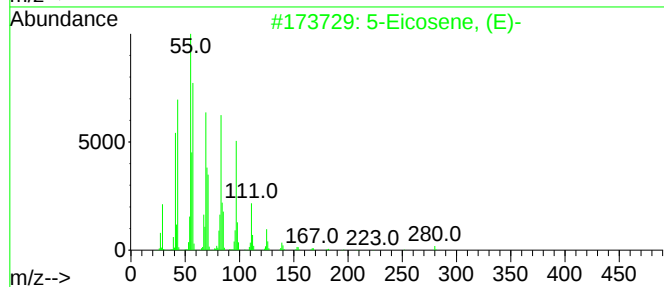
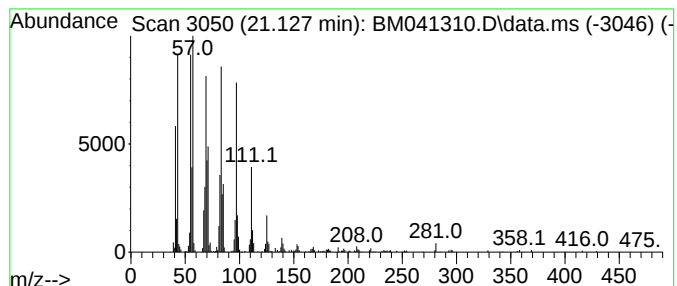
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	4.16 ng	440130	Chrysene-d12	21.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Eicosene, (E)-	280	C20H40	074685-30-6	95
2			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
3			Behenic alcohol	326	C22H46O	000661-19-8	94
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080723\
Data File : BM041310.D
Acq On : 07 Aug 2023 13:43
Operator : MA/JU
Sample : 03903-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.899	2.1	ng	73342	1	7.787	703012	20.0
Hexathiane	15.133	7.2	ng	537467	3	14.457	1489160	20.0
Benzophenone	15.827	3.0	ng	226078	3	14.457	1489160	20.0
n-Hexadecanoic ...	18.115	18.3	ng	1795510	4	17.215	1964170	20.0
Octadecanoic acid	19.398	7.7	ng	817214	5	21.421	2115270	20.0
5-Eicosene, (E)-	21.127	4.2	ng	440130	5	21.421	2115270	20.0