

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040225\
 Data File : BM049792.D
 Acq On : 02 Apr 2025 16:04
 Operator : RC/JU
 Sample : Q1681-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TP-12

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-BM031325.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM049792.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.016	3	5	19	rVB	103637	151898	1.29%	0.259%
2	4.904	320	326	336	rBV	580241	789518	6.71%	1.349%
3	5.369	398	405	420	rBV	3953666	5401287	45.91%	9.226%
4	6.957	668	675	690	rBV	3755968	5597436	47.58%	9.561%
5	7.787	809	816	824	rVB	977793	1486535	12.64%	2.539%
6	8.940	1004	1012	1020	rBV	2129540	3313614	28.17%	5.660%
7	10.581	1283	1291	1303	rVB	1148831	1836252	15.61%	3.137%
8	13.051	1704	1711	1718	rBV	5607333	7790339	66.22%	13.307%
9	14.427	1935	1945	1954	rBV	1644047	2408334	20.47%	4.114%
10	15.786	2171	2176	2183	rBV	241088	317546	2.70%	0.542%
11	15.916	2191	2198	2216	rBV	4396597	6004446	51.04%	10.257%
12	17.168	2404	2411	2417	rBV	2028894	2747087	23.35%	4.693%
13	18.068	2559	2564	2572	rBV	376642	581722	4.94%	0.994%
14	19.351	2777	2782	2789	rBV2	104158	176921	1.50%	0.302%
15	19.792	2852	2857	2864	rBV	11106560	11764708	100.00%	20.096%
16	20.486	2971	2975	2987	rVB	588832	727872	6.19%	1.243%
17	21.092	3074	3078	3089	rBV2	243631	417096	3.55%	0.712%
18	21.398	3125	3130	3136	rBV	2397290	3460070	29.41%	5.910%
19	24.397	3632	3640	3661	rVB	1414175	3569396	30.34%	6.097%

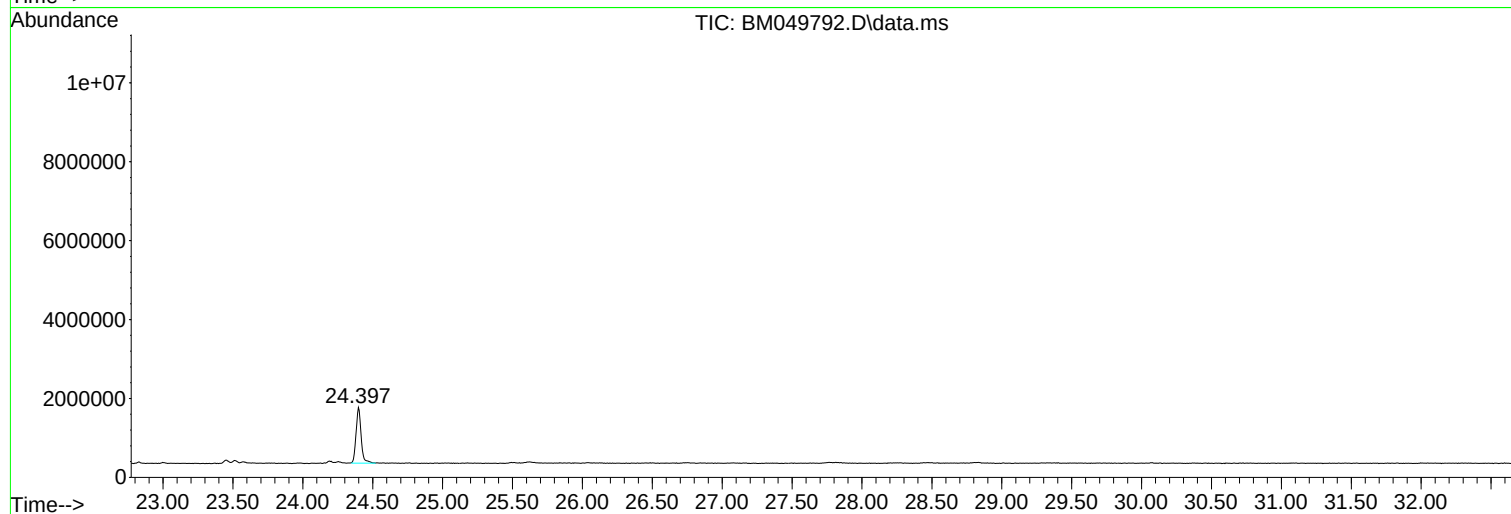
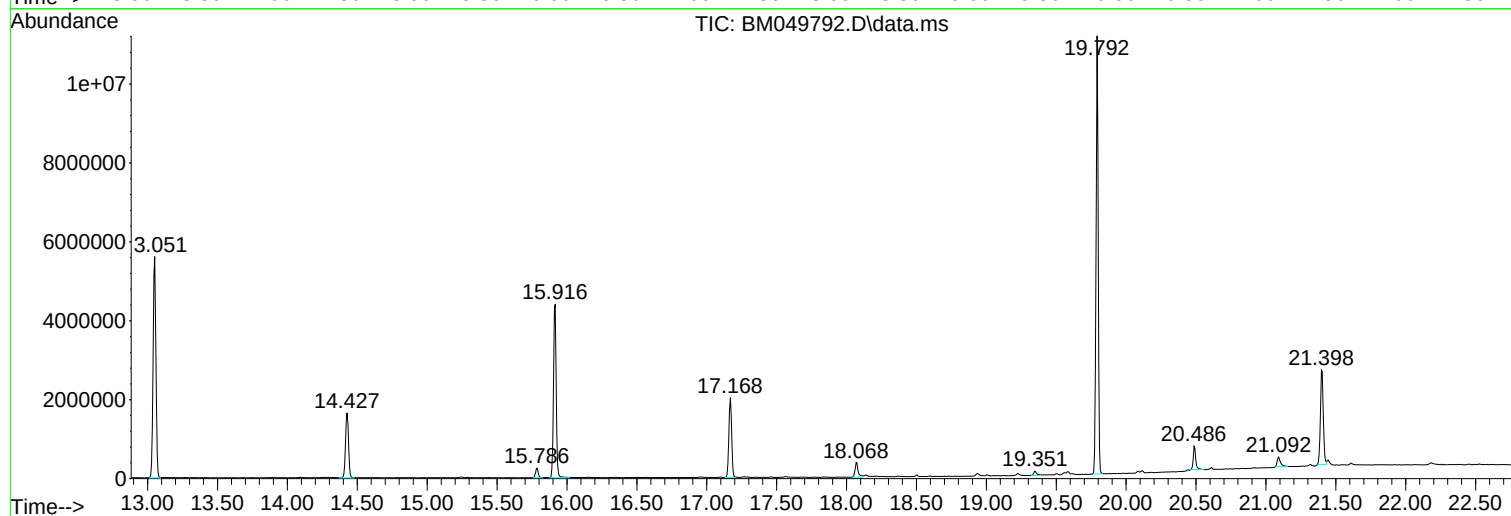
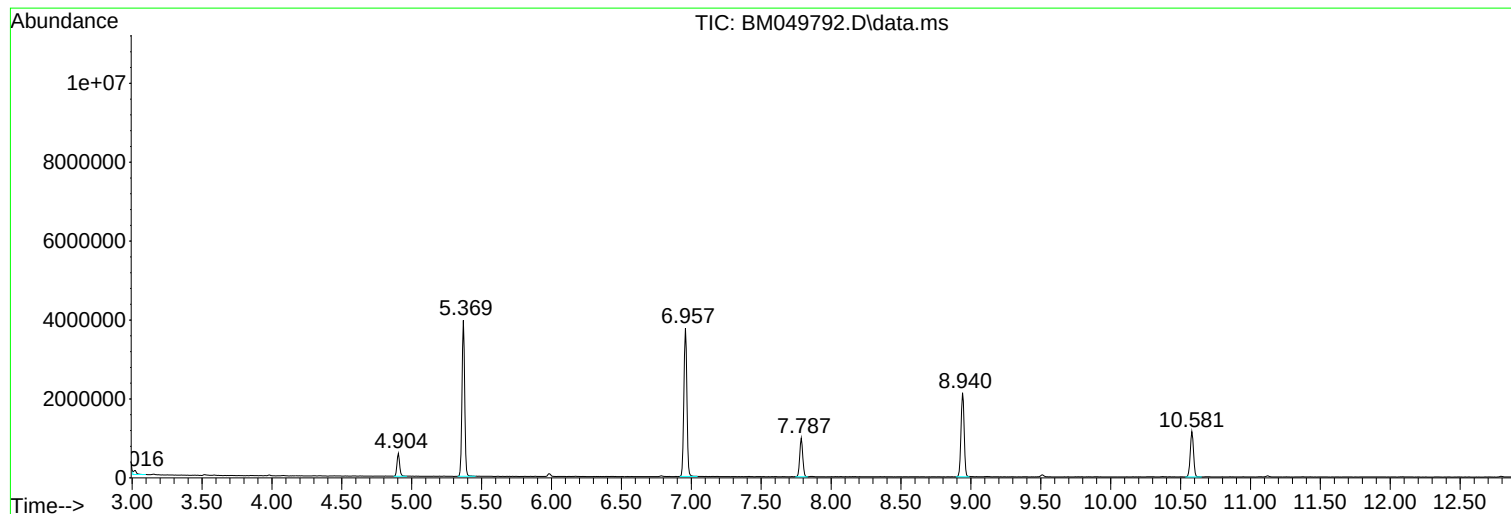
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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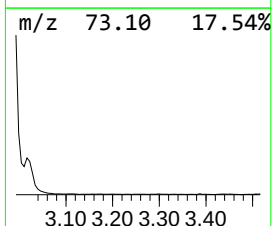
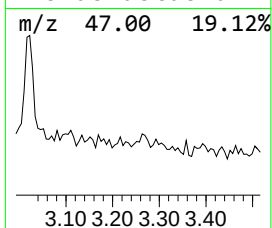
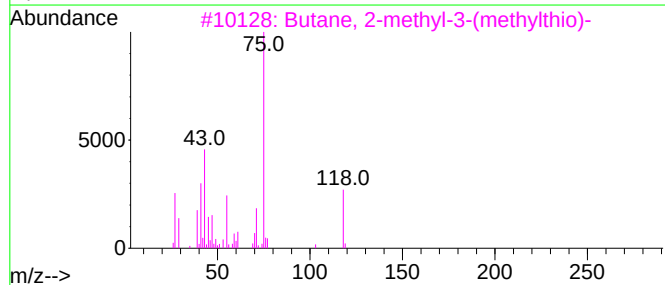
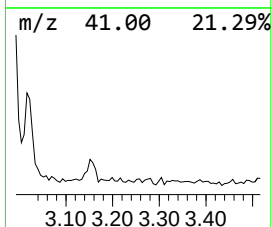
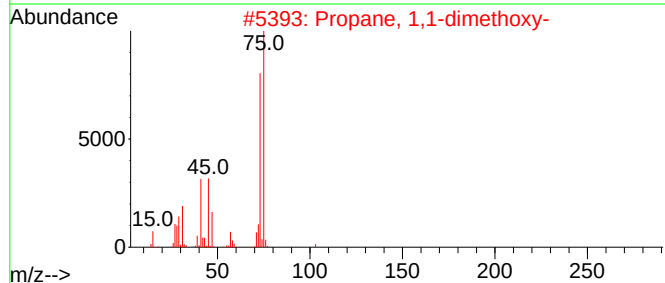
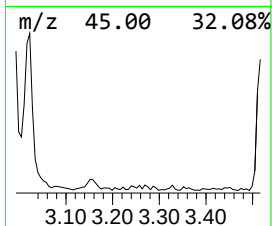
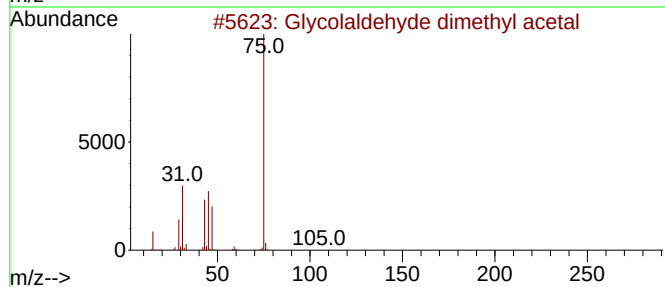
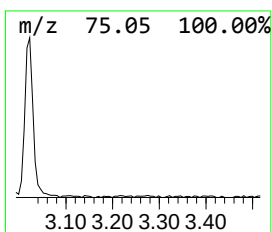
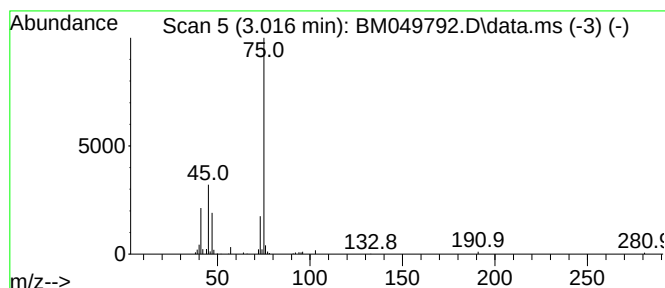
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Glycolaldehyde dimethyl acetal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.016	2.04 ng	151898	1,4-Dichlorobenzene-d4	7.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	56
2			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	40
3			Butane, 2-methyl-3-(methylthio)-	118	C6H14S	053897-51-1	39
4			Ethane, 2-chloro-1,1-dimethoxy-	124	C4H9ClO2	000097-97-2	36
5			3-Bromopropionaldehyde dimethyl ...	182	C5H11BrO2	036255-44-4	36



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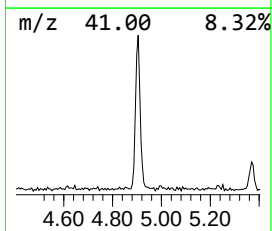
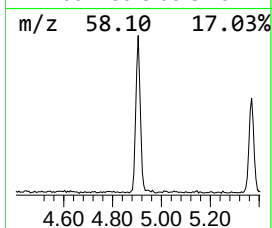
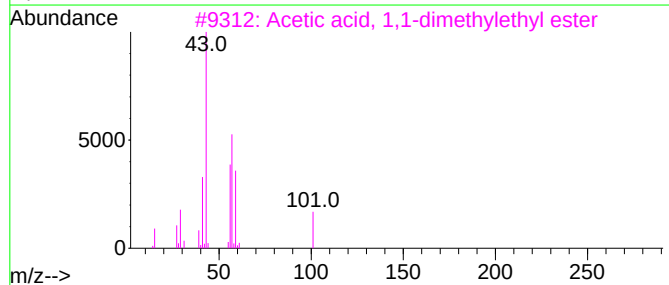
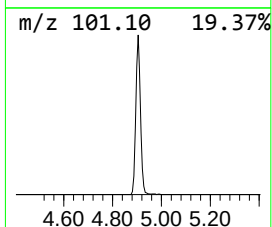
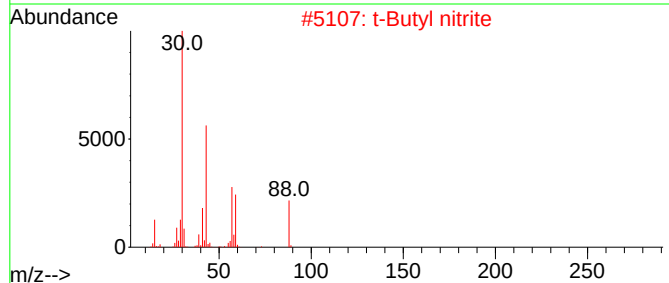
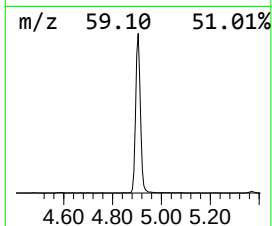
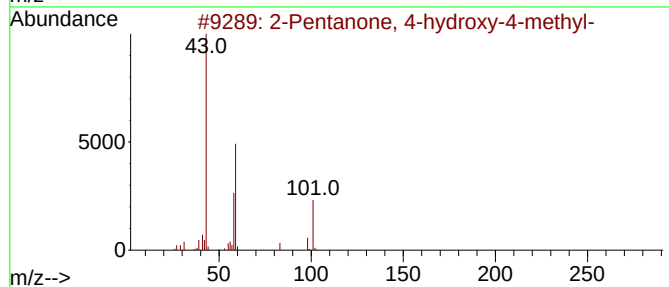
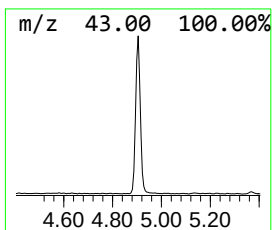
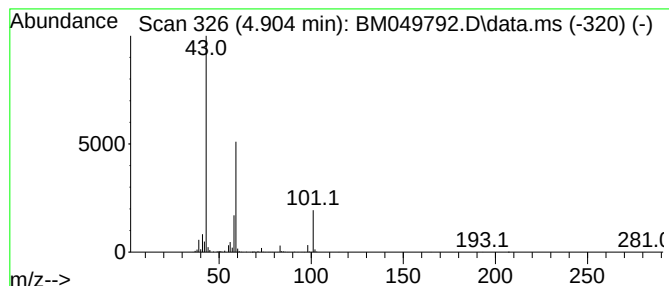
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.904	10.62 ng	789518	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	50		
2	t-Butyl nitrite	103	C4H9NO2	000540-80-7	42		
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
4	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		



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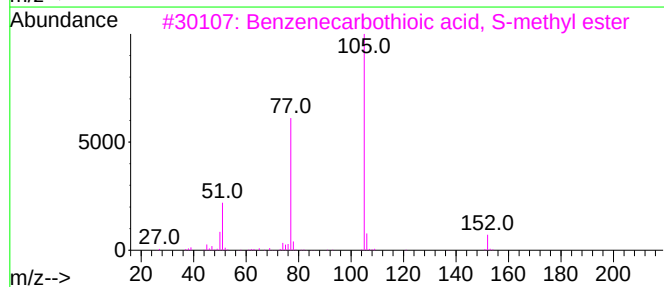
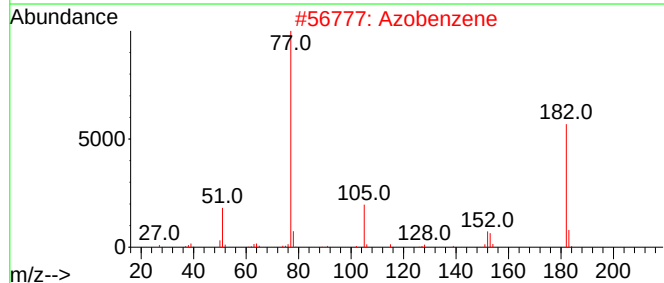
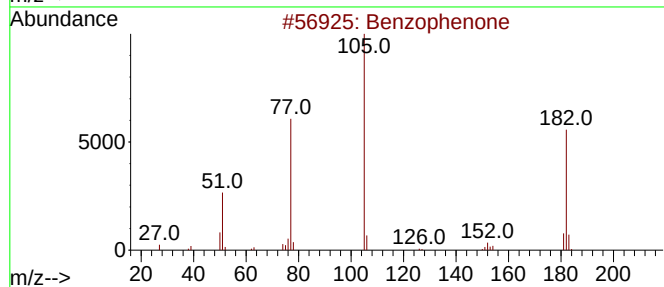
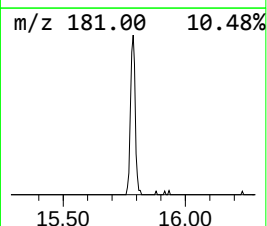
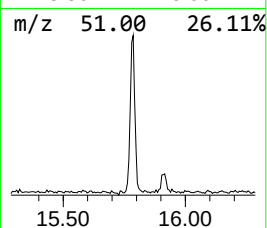
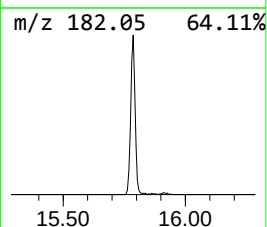
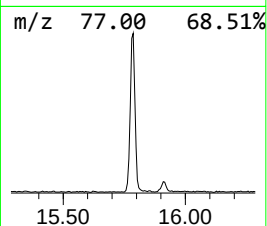
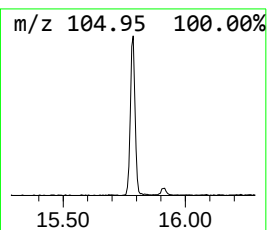
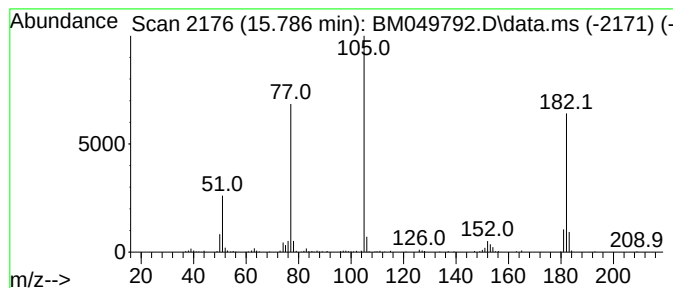
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Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.786	2.64 ng	317546	Acenaphthene-d10	14.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	59
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	46
5			Benzoylformic acid	150	C8H6O3	000611-73-4	46



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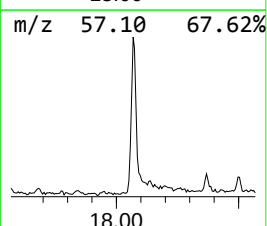
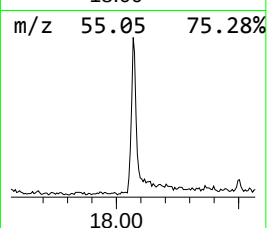
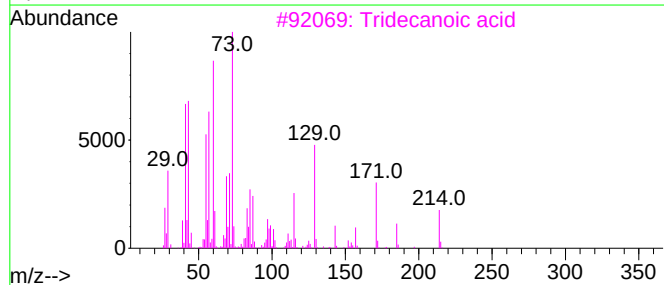
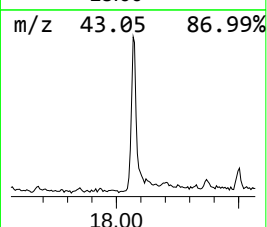
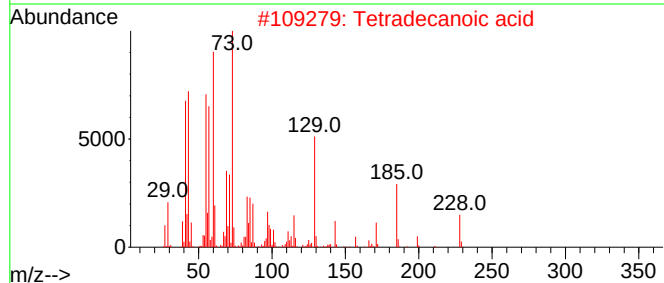
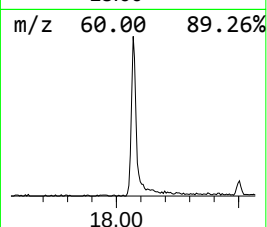
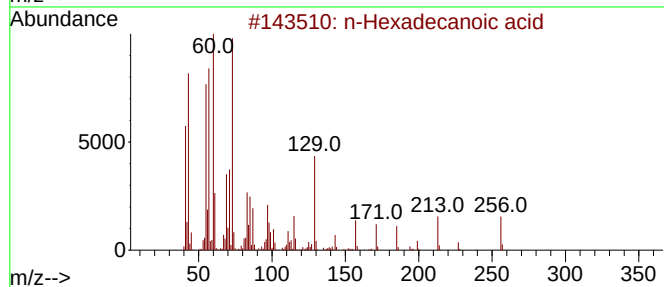
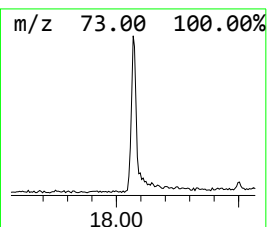
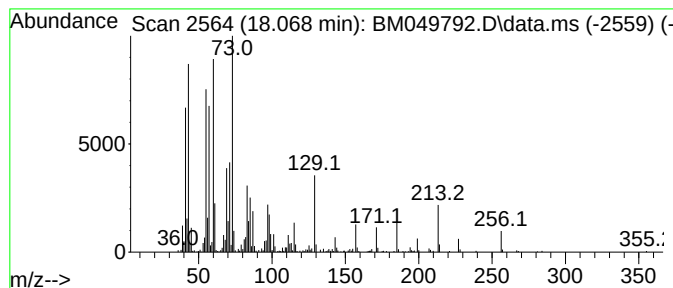
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.068	4.24 ng	581722	Phenanthrene-d10	17.168

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	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Octadecanoic acid	284	C18H36O2	000057-11-4	80
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	68



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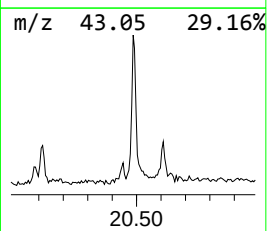
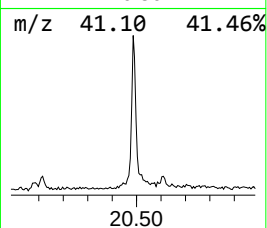
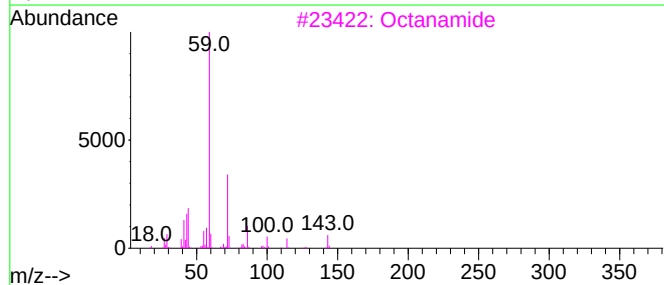
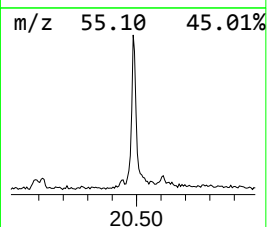
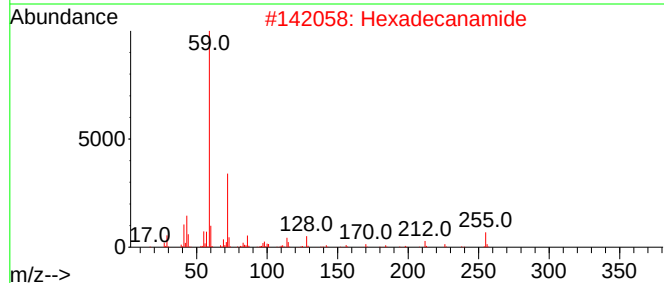
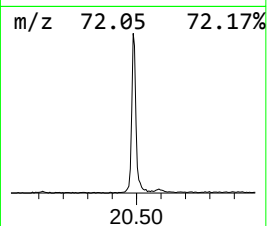
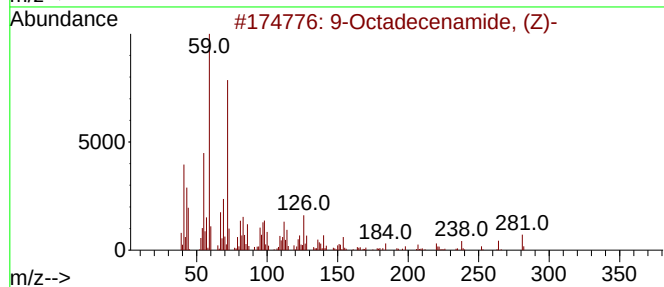
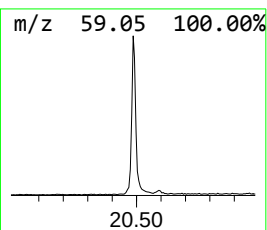
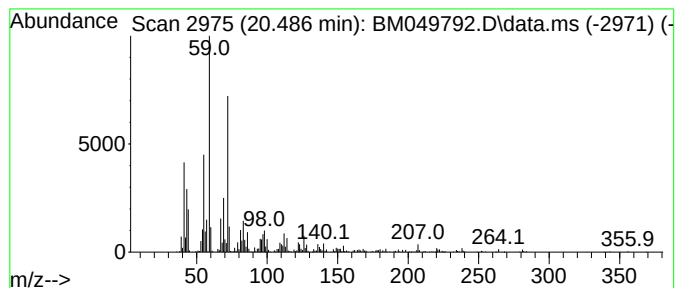
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.486	4.21 ng	727872	Chrysene-d12	21.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2			Hexadecanamide	255	C16H33NO	000629-54-9	72
3			Octanamide	143	C8H17NO	000629-01-6	59
4			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	50
5			Diazene, [1-(2,2-dimethylhydrazi...	172	C8H20N4	061940-94-1	47



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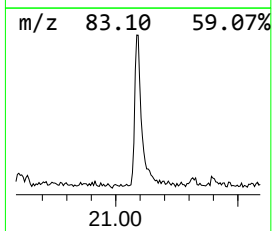
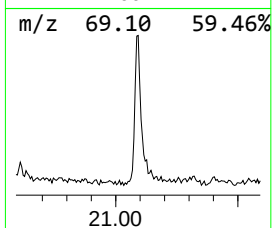
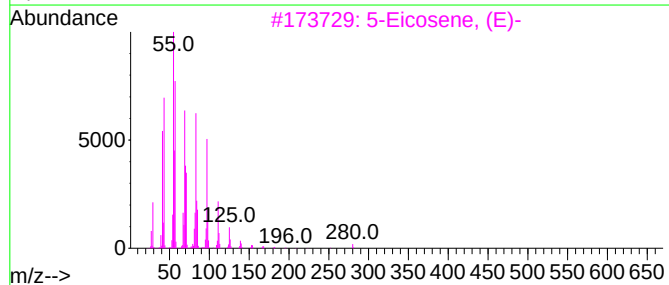
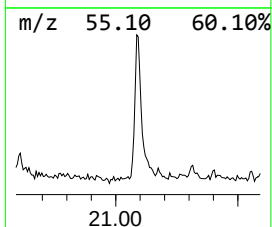
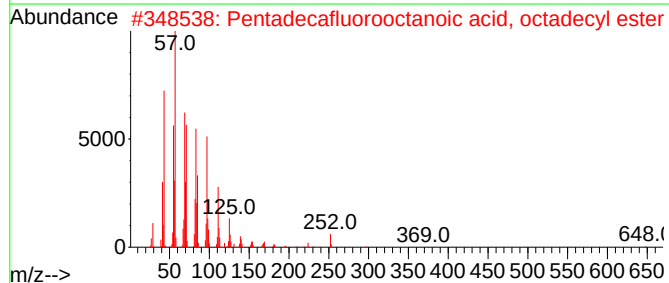
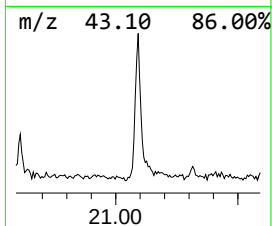
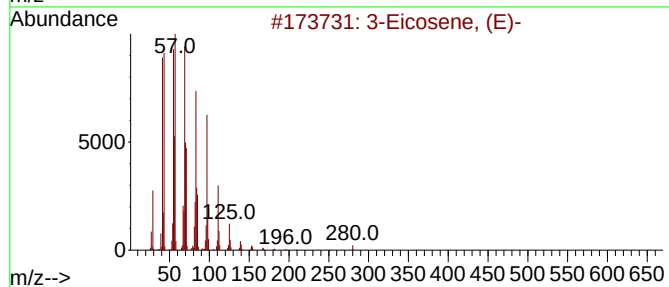
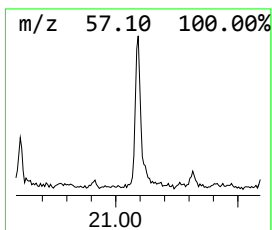
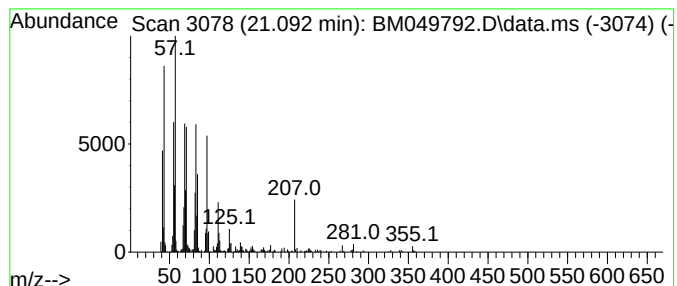
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 3-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.092	2.41 ng	417096	Chrysene-d12	21.398

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Eicosene, (E)-	280	C20H40	074685-33-9	95
2		Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	87
3		5-Eicosene, (E)-	280	C20H40	074685-30-6	86
4		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	83
5		Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040225\
Data File : BM049792.D
Acq On : 02 Apr 2025 16:04
Operator : RC/JU
Sample : Q1681-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Glycolaldehyde ...	3.016	2.0	ng	151898	1	7.787	1486540	20.0
2-Pentanone, 4-...	4.904	10.6	ng	789518	1	7.787	1486540	20.0
Benzophenone	15.786	2.6	ng	317546	3	14.427	2408330	20.0
n-Hexadecanoic ...	18.068	4.2	ng	581722	4	17.168	2747090	20.0
9-Octadecenamid...	20.486	4.2	ng	727872	5	21.398	3460070	20.0
3-Eicosene, (E)-	21.092	2.4	ng	417096	5	21.398	3460070	20.0