

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082824\
 Data File : BM047378.D
 Acq On : 28 Aug 2024 13:03
 Operator : RC/JU
 Sample : P3739-13
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 WC-3

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-BM082624.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047378.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.252	59	62	76	rVB	215457	306942	2.96%	0.496%
2	4.557	277	284	293	rVB	196987	283018	2.73%	0.457%
3	5.010	354	361	379	rBV	2808619	4257314	41.04%	6.874%
4	6.569	619	626	641	rBV	2848050	4583724	44.19%	7.401%
5	6.981	691	696	705	rBV	78614	143321	1.38%	0.231%
6	7.346	750	758	767	rBV	896178	1391208	13.41%	2.246%
7	8.498	945	954	966	rBV	1853547	3053046	29.43%	4.930%
8	10.104	1219	1227	1238	rBV	1115018	1925518	18.56%	3.109%
9	10.869	1349	1357	1372	rBV	161758	360301	3.47%	0.582%
10	12.616	1646	1654	1673	rBV	4608054	7161755	69.04%	11.564%
11	14.010	1884	1891	1906	rVB	1850373	2754657	26.55%	4.448%
12	14.245	1924	1931	1932	rBV	1638078	1972912	19.02%	3.186%
13	14.263	1932	1934	1946	rVB	1902525	2427245	23.40%	3.919%
14	15.521	2141	2148	2159	rBV	4145167	6099969	58.80%	9.849%
15	16.774	2355	2361	2368	rBV	2279625	3361196	32.40%	5.427%
16	16.910	2380	2384	2393	rVB3	93754	144151	1.39%	0.233%
17	17.710	2515	2520	2529	rBV	877967	1413998	13.63%	2.283%
18	18.257	2609	2613	2622	rVB2	84009	127764	1.23%	0.206%
19	18.857	2711	2715	2720	rBV	137738	208703	2.01%	0.337%
20	19.015	2737	2742	2759	rBV	406607	836850	8.07%	1.351%
21	19.192	2769	2772	2775	rBV2	129698	183869	1.77%	0.297%
22	19.221	2775	2777	2783	rVB	125221	185356	1.79%	0.299%
23	19.445	2809	2815	2820	rBV	8744676	10373411	100.00%	16.749%
24	20.751	3033	3037	3043	rBV	608379	806120	7.77%	1.302%
25	20.956	3069	3072	3076	rBV	133992	158032	1.52%	0.255%
26	21.021	3077	3083	3087	rVV	2562163	3787865	36.52%	6.116%
27	21.062	3087	3090	3098	rVB	333967	507026	4.89%	0.819%
28	23.721	3535	3542	3553	rVB	1320507	3117677	30.05%	5.034%

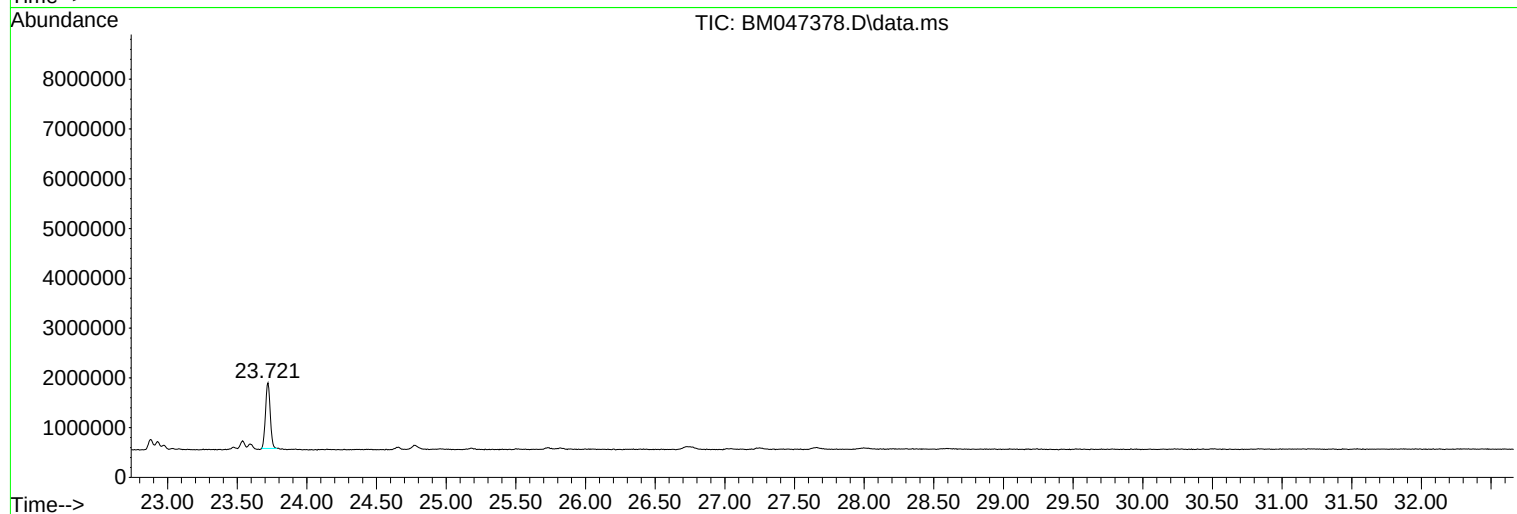
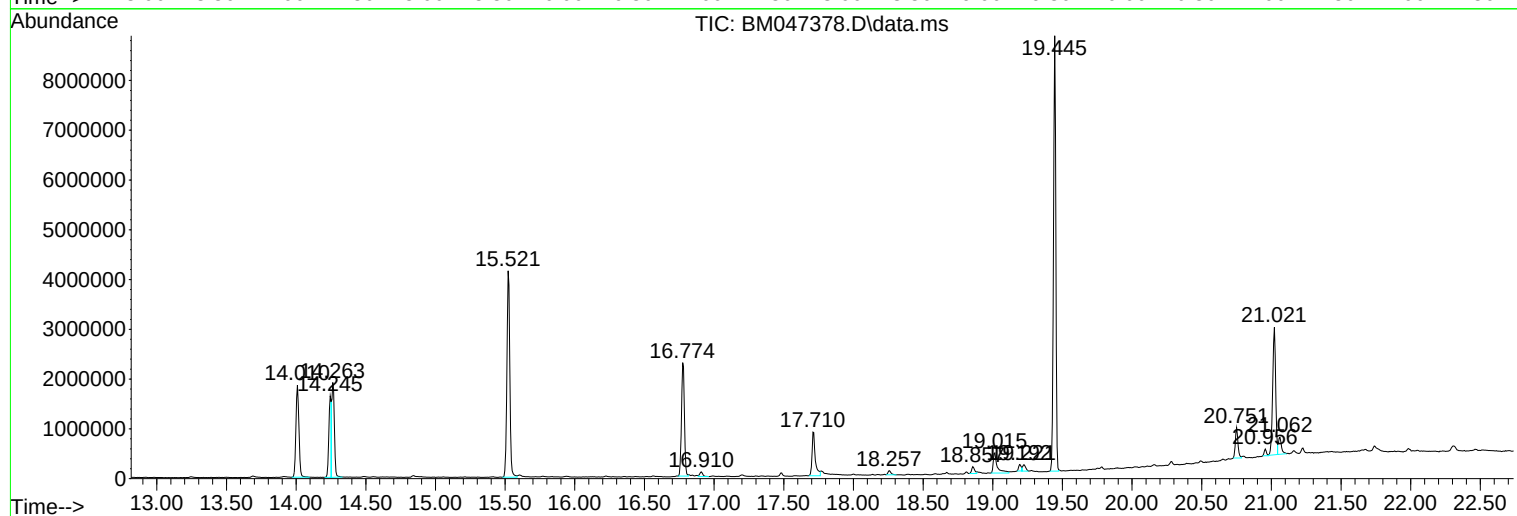
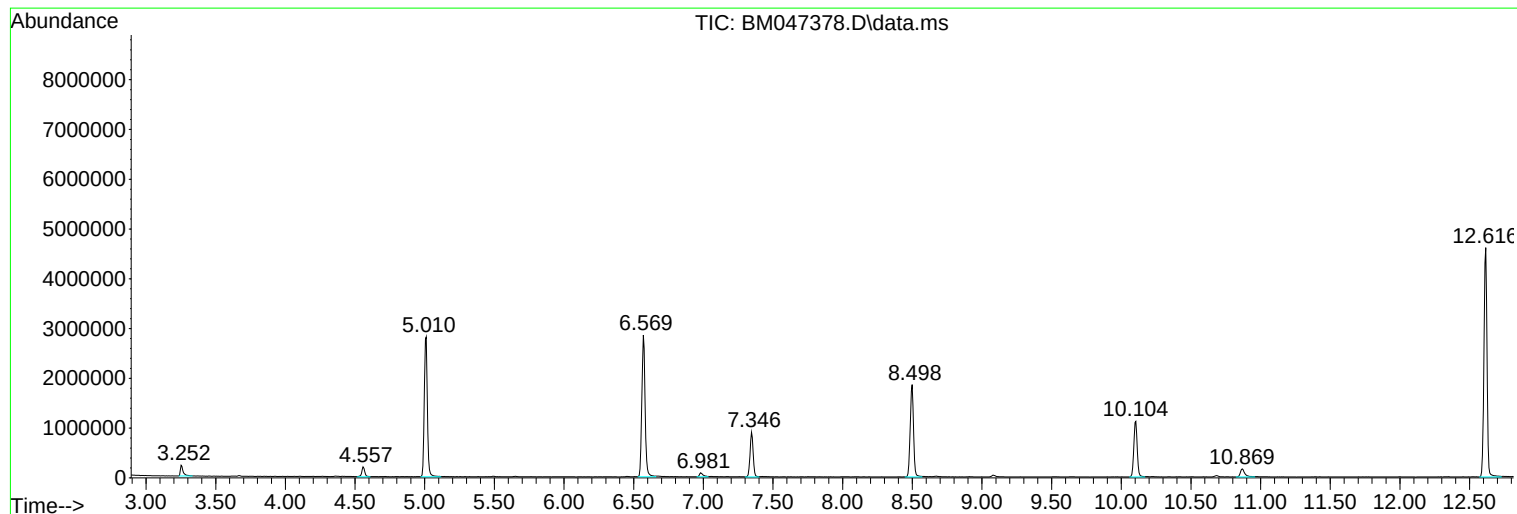
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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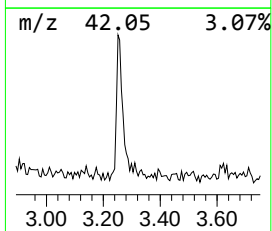
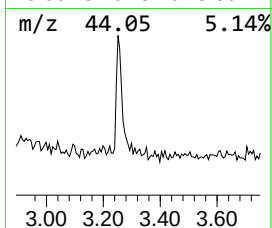
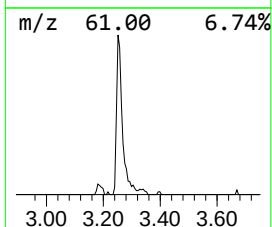
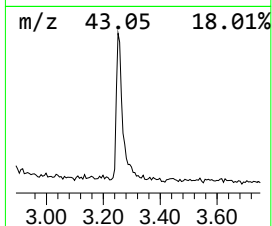
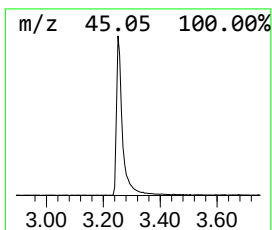
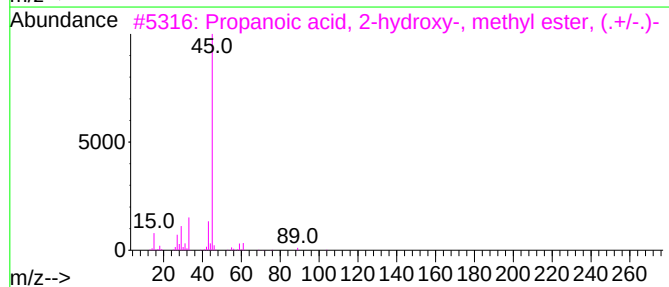
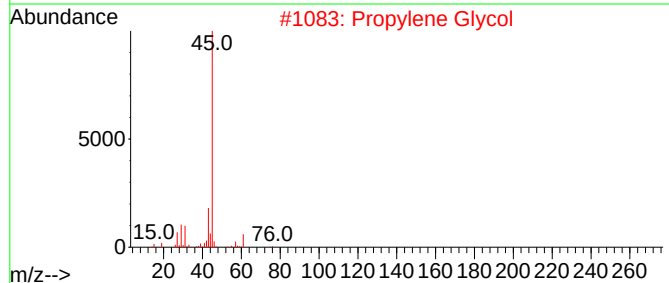
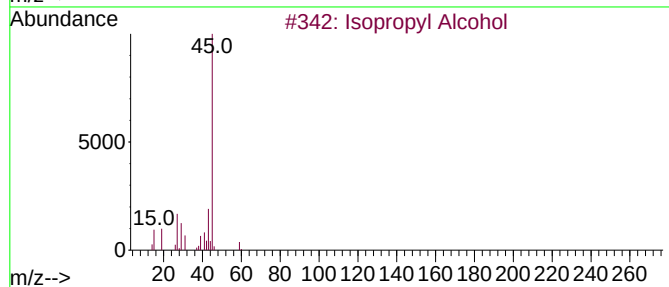
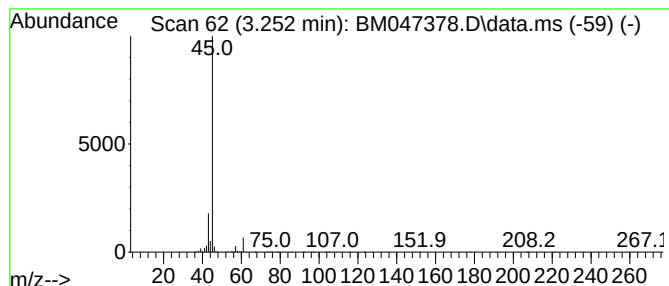
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.252	4.41 ng	306942	1,4-Dichlorobenzene-d4	7.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
2			Propylene Glycol	76	C3H8O2	000057-55-6	46
3			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
4			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
5			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9



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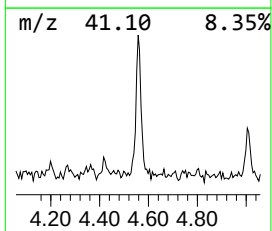
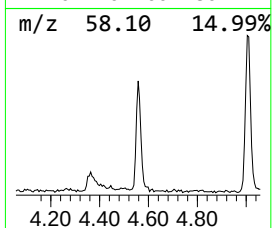
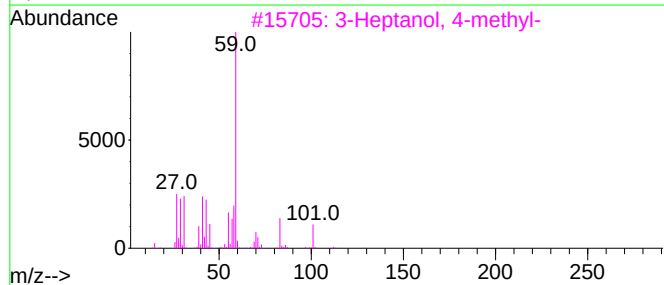
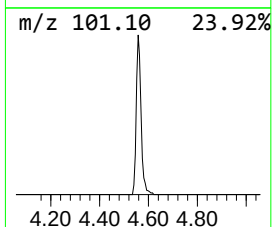
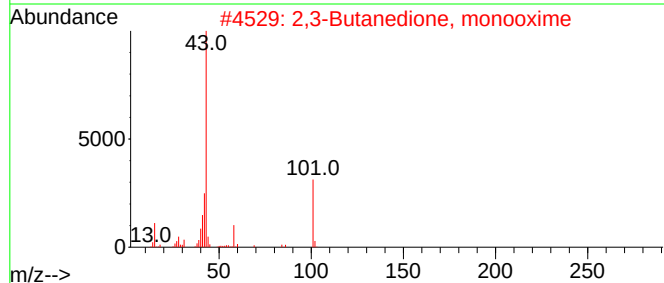
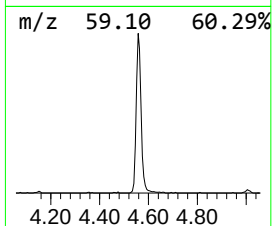
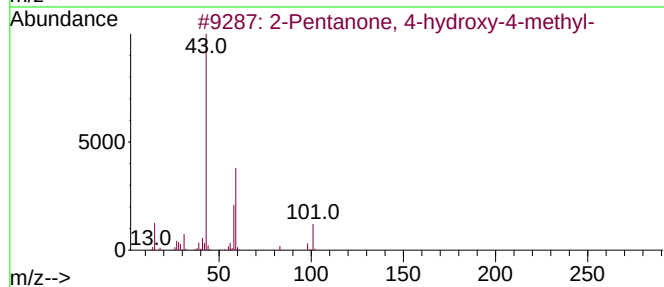
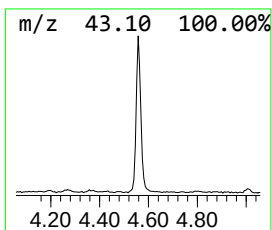
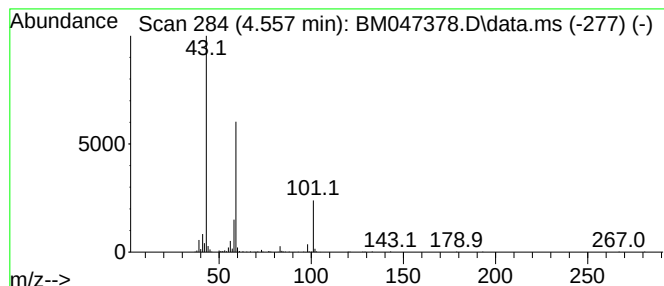
Instrument :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD			R.T.
4.557	4.07 ng	283018	1,4-Dichlorobenzene-d4			7.346
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	25
3	3-Heptanol, 4-methyl-		130	C8H18O	014979-39-6	25
4	1,3-Dioxolane-2-methanol, 2,4-di...		132	C6H12O3	053951-43-2	25
5	Tetraglyme		222	C10H22O5	000143-24-8	23



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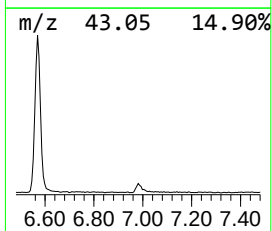
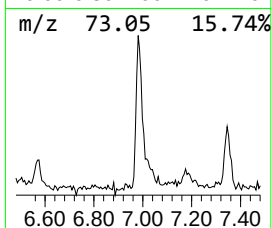
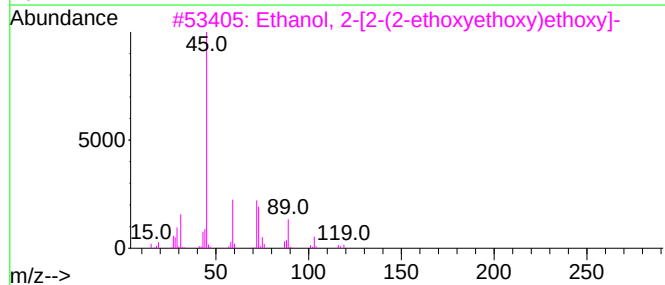
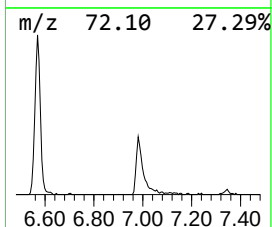
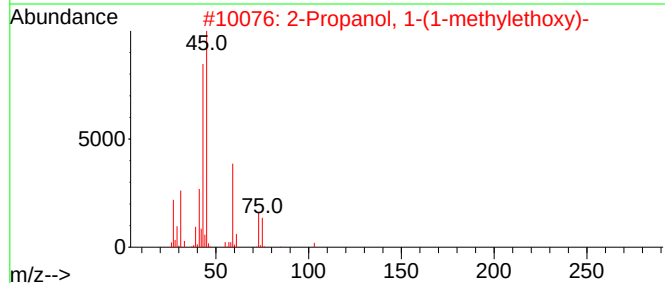
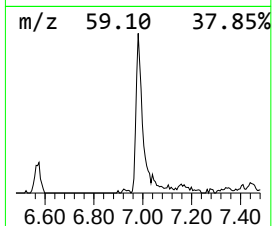
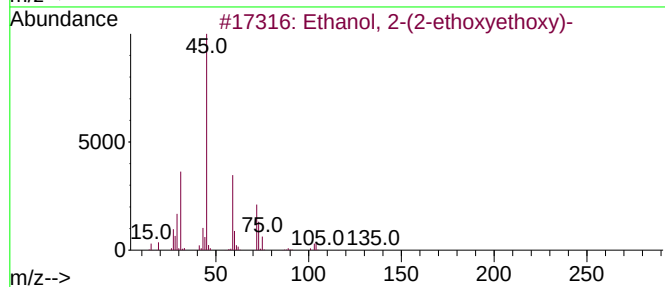
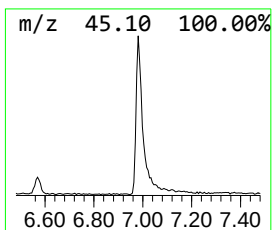
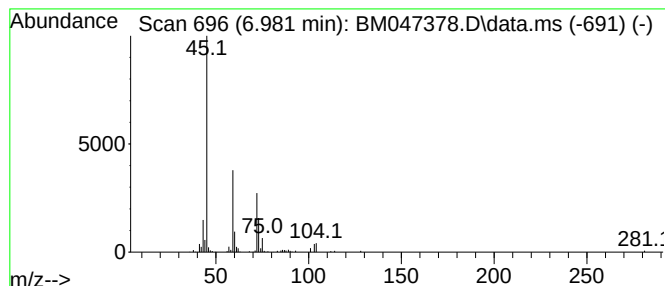
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.981	2.06 ng	143321	1,4-Dichlorobenzene-d4	7.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
3			Ethanol, 2-[2-(2-ethoxyethoxy)et...]	178	C8H18O4	000112-50-5	45
4			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42
5			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	38



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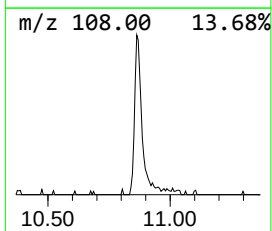
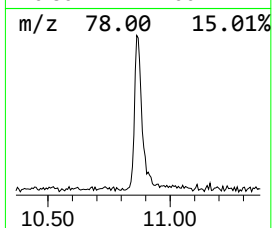
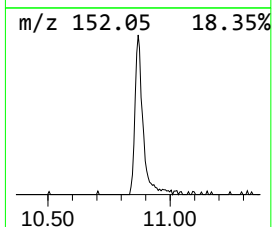
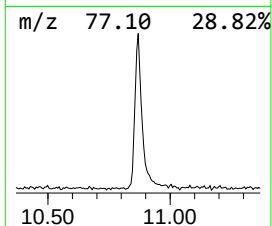
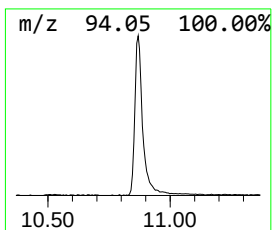
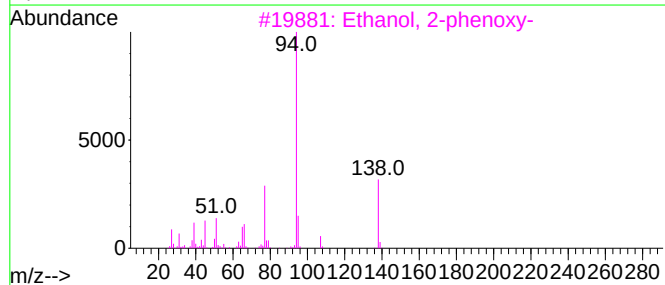
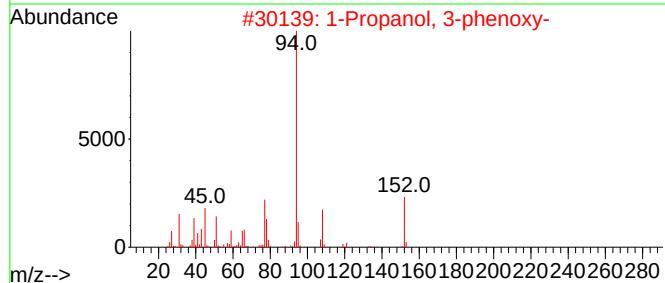
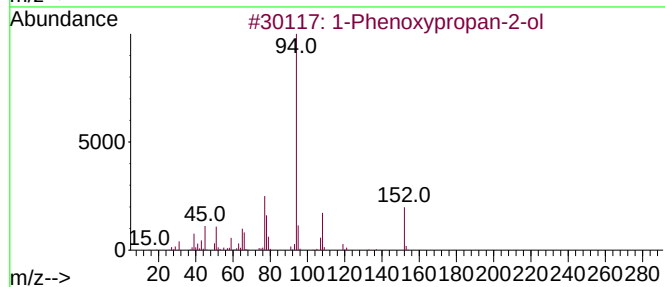
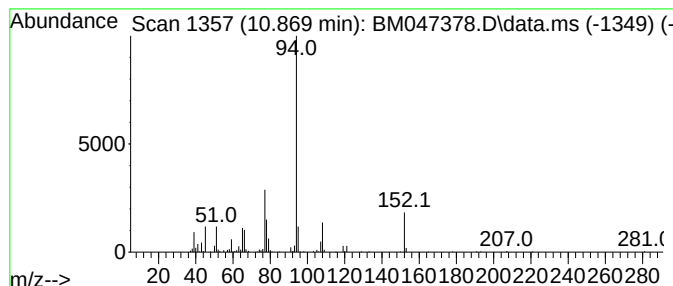
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Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.869	3.74 ng	360301	Naphthalene-d8	10.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
5			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59



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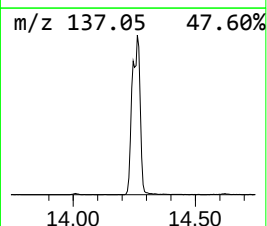
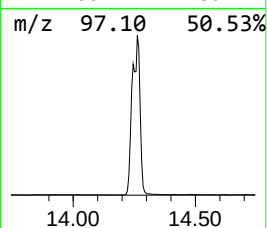
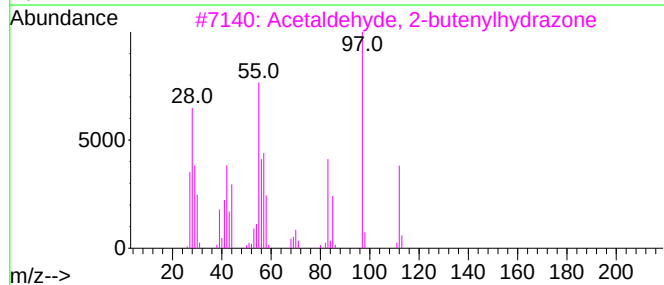
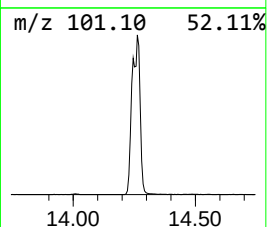
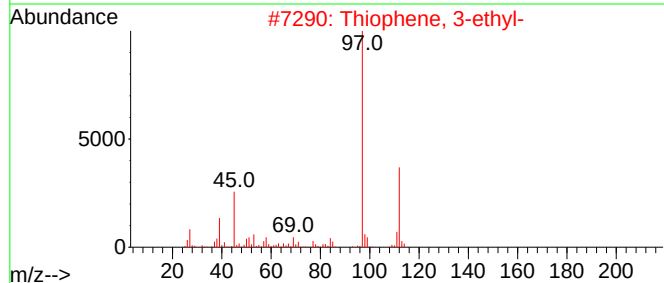
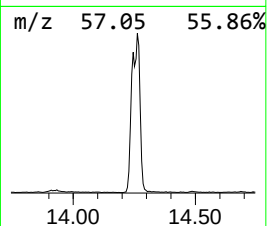
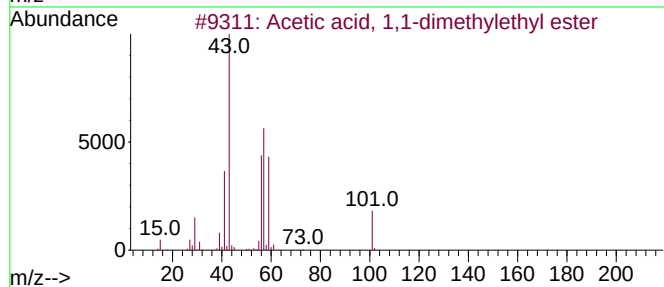
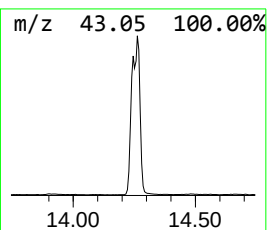
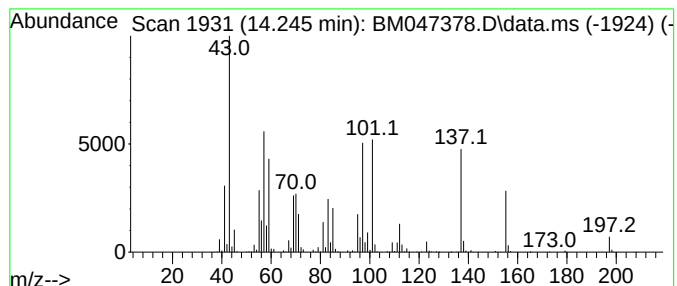
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown14.245 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.245	14.32 ng	1972910	Acenaphthene-d10	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	14
2			Thiophene, 3-ethyl-	112	C6H8S	001795-01-3	11
3			Acetaldehyde, 2-butenylhydrazone	112	C6H12N2	075268-07-4	11
4			Octyl (E)-2-methylbut-2-enoate	212	C13H24O2	1000373-71-2	10
5			Butyl decyl ether	214	C14H30O	1000406-40-2	10



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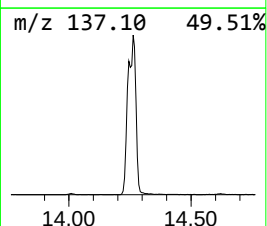
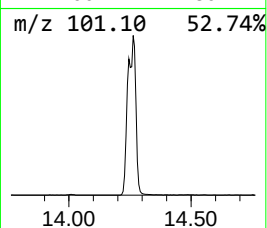
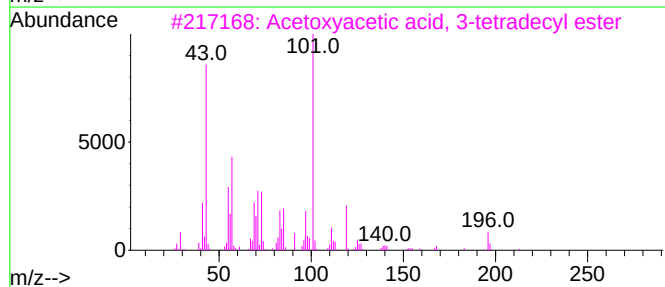
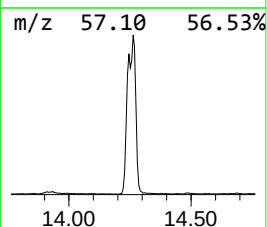
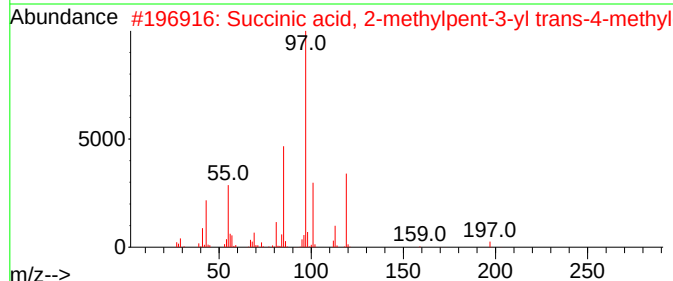
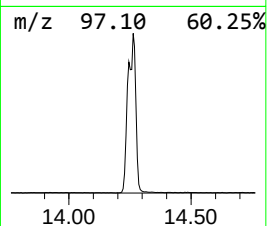
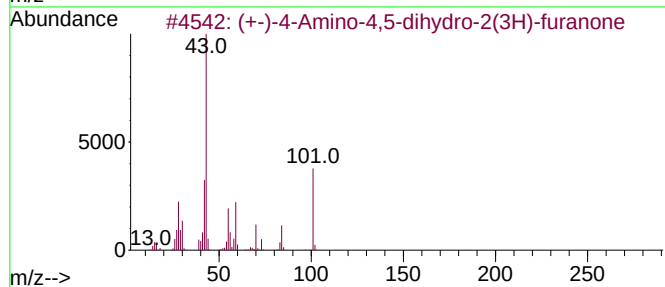
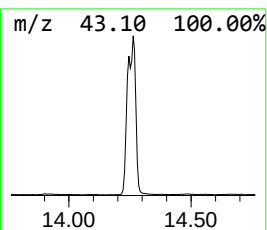
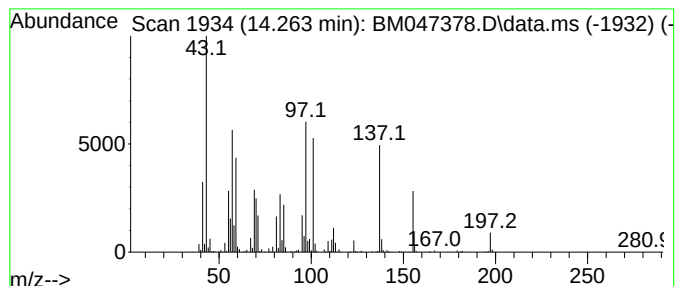
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.263 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.263	17.62 ng	2427250	Acenaphthene-d10	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7N02	016504-58-8	22		
2	Succinic acid, 2-methylpent-3-yl...	298	C17H30O4	1000390-06-8	14		
3	Acetoxyacetic acid, 3-tetradecyl...	314	C18H34O4	1000308-80-8	14		
4	Hexadecane, 1-bromo-	304	C16H33Br	000112-82-3	14		
5	Acetaldehyde, 2-butenylhydrazone	112	C6H12N2	075268-07-4	14		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082824\
Data File : BM047378.D
Acq On : 28 Aug 2024 13:03
Operator : RC/JU
Sample : P3739-13
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-3

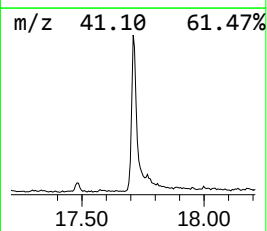
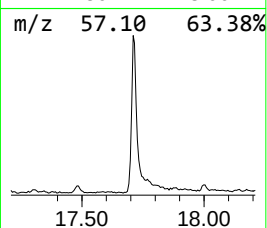
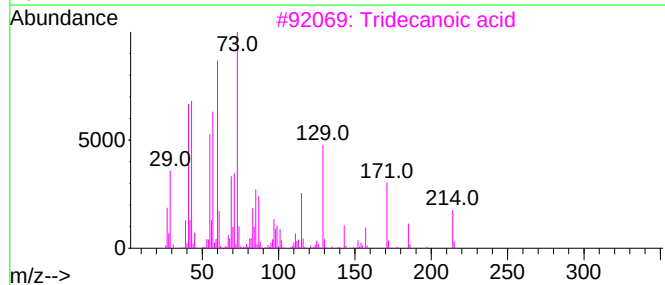
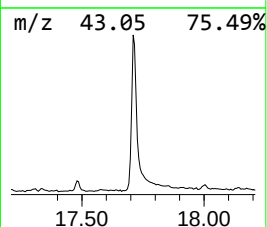
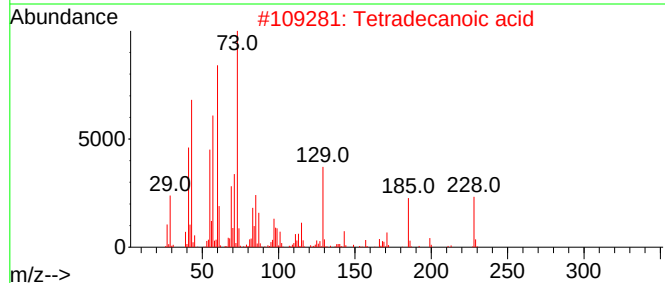
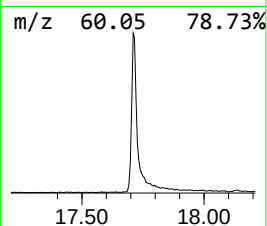
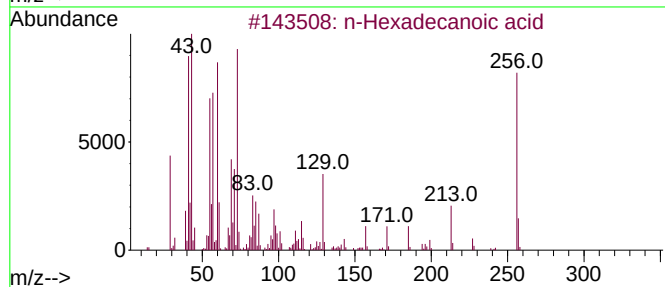
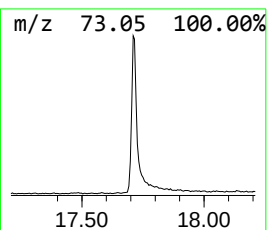
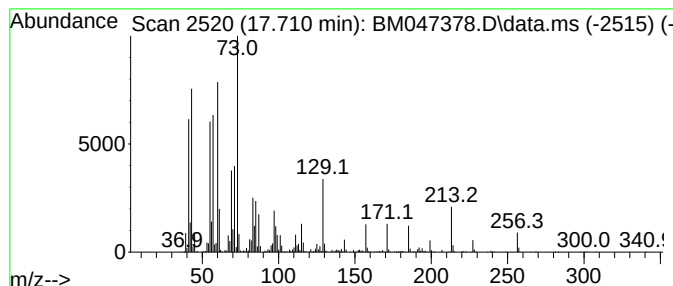
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.709	8.41 ng	1414000	Phenanthrene-d10	16.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	91
4			Octadecanoic acid	284	C18H36O2	000057-11-4	87
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082824\
Data File : BM047378.D
Acq On : 28 Aug 2024 13:03
Operator : RC/JU
Sample : P3739-13
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-3

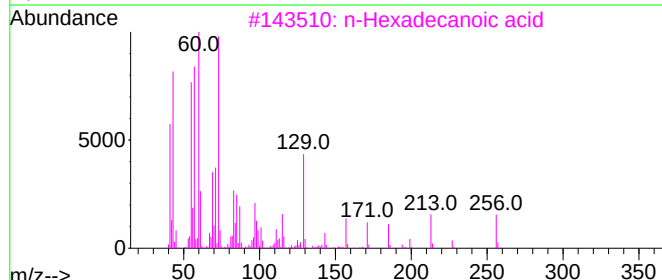
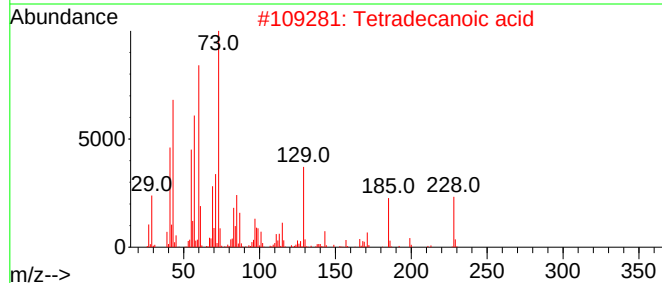
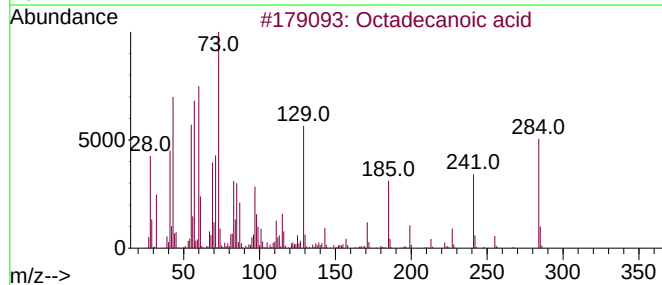
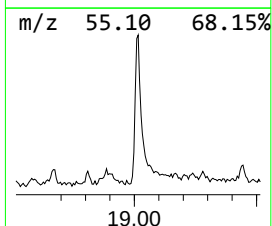
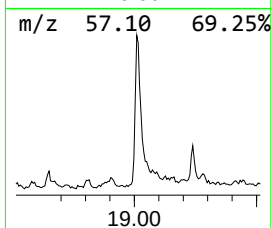
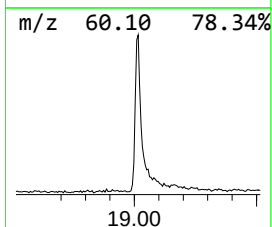
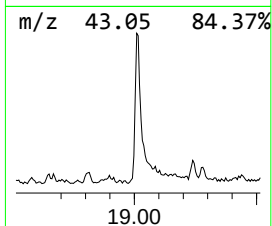
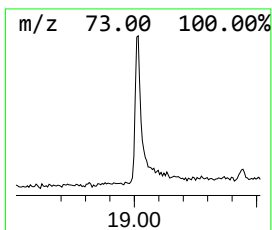
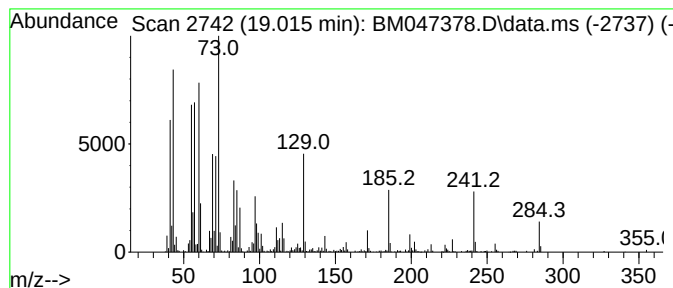
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.015	4.42 ng	836850	Chrysene-d12	21.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5			Tridecanoic acid	214	C13H26O2	000638-53-9	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082824\
Data File : BM047378.D
Acq On : 28 Aug 2024 13:03
Operator : RC/JU
Sample : P3739-13
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-3

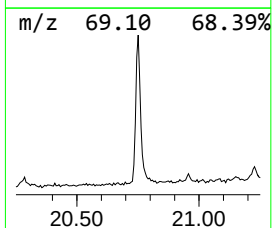
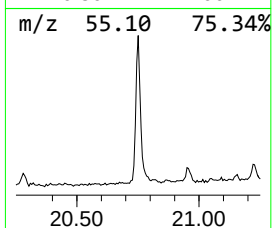
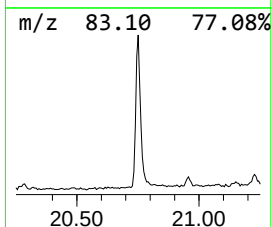
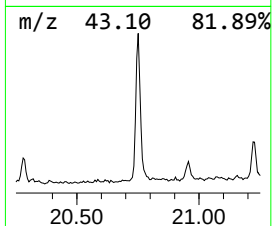
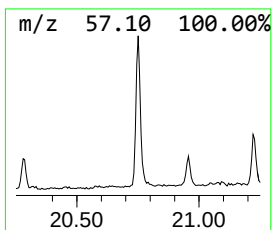
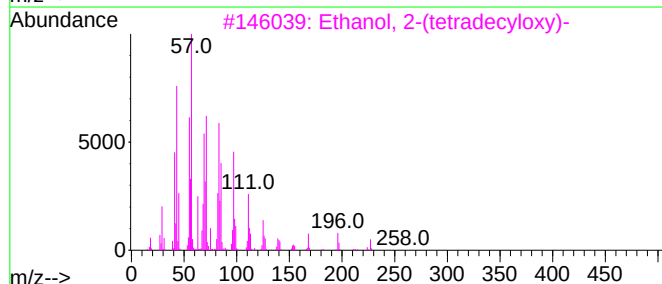
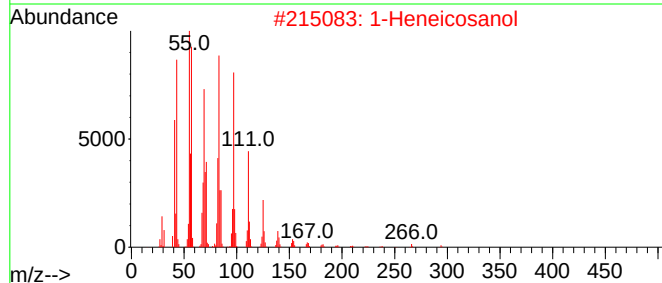
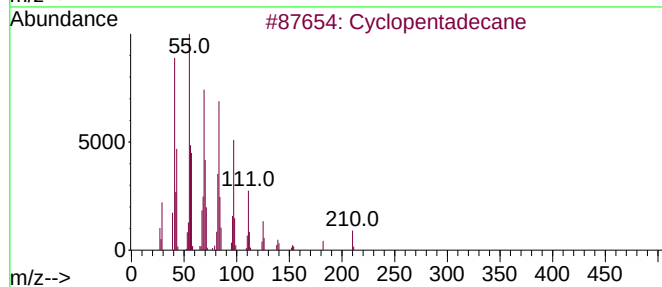
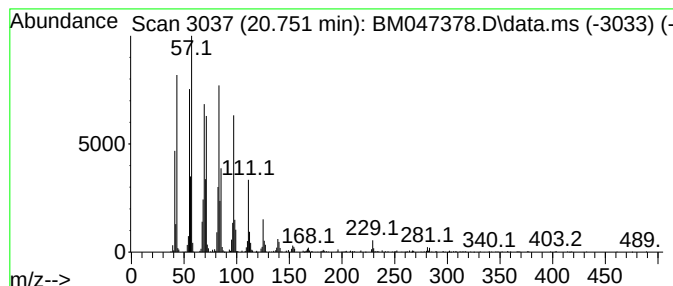
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclopentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.750	4.26 ng	806120	Chrysene-d12	21.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	93
2			1-Heneicosanol	312	C21H44O	015594-90-8	93
3			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082824\
Data File : BM047378.D
Acq On : 28 Aug 2024 13:03
Operator : RC/JU
Sample : P3739-13
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.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
Isopropyl Alcohol	3.252	4.4	ng	306942	1	7.346	1391210	20.0
2-Pentanone, 4-...	4.557	4.1	ng	283018	1	7.346	1391210	20.0
Ethanol, 2-(2-e...	6.981	2.1	ng	143321	1	7.346	1391210	20.0
1-Phenoxypropan...	10.869	3.7	ng	360301	2	10.104	1925520	20.0
unknown14.245	14.245	14.3	ng	1972910	3	14.010	2754660	20.0
unknown14.263	14.263	17.6	ng	2427250	3	14.010	2754660	20.0
n-Hexadecanoic ...	17.709	8.4	ng	1414000	4	16.774	3361200	20.0
Octadecanoic acid	19.015	4.4	ng	836850	5	21.021	3787870	20.0
Cyclopentadecane	20.750	4.3	ng	806120	5	21.021	3787870	20.0