

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM050725\
 Data File : BM050134.D
 Acq On : 07 May 2025 14:26
 Operator : RC/JU
 Sample : Q1945-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 GB1W

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-BM042825.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM050134.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.863	314	319	331	rVB	208240	310157	1.61%	0.384%
2	5.340	393	400	415	rBV	2385945	3770258	19.55%	4.663%
3	6.940	665	672	699	rBV	1132890	2400630	12.45%	2.969%
4	7.746	799	809	816	rBV	922189	1502810	7.79%	1.859%
5	8.904	998	1006	1023	rBV	2695910	4799196	24.88%	5.935%
6	10.328	1241	1248	1269	rBV	537750	1312818	6.81%	1.624%
7	10.540	1277	1284	1297	rBV	1075868	1918339	9.95%	2.372%
8	11.516	1438	1450	1477	rBV	2231038	5625961	29.17%	6.958%
9	13.010	1697	1704	1722	rBV	8445469	12165948	63.08%	15.046%
10	14.392	1933	1939	1956	rVB	1779670	2743703	14.23%	3.393%
11	15.757	2165	2171	2182	rBV	352981	520261	2.70%	0.643%
12	15.892	2187	2194	2216	rBV	6964284	10602956	54.98%	13.113%
13	16.598	2309	2314	2321	rVB	441338	616059	3.19%	0.762%
14	17.145	2401	2407	2420	rBV	2197050	3170702	16.44%	3.921%
15	18.045	2554	2560	2568	rBV	1487258	2215520	11.49%	2.740%
16	19.321	2773	2777	2789	rBV	484335	839837	4.35%	1.039%
17	19.674	2834	2837	2844	rBV	151479	193997	1.01%	0.240%
18	19.774	2848	2854	2862	rVB	16012713	19286006	100.00%	23.851%
19	20.515	2978	2980	2987	rVB	206589	207304	1.07%	0.256%
20	21.392	3124	3129	3135	rBV	2282621	3267112	16.94%	4.041%
21	24.386	3632	3638	3649	rVB	1351096	3389325	17.57%	4.192%

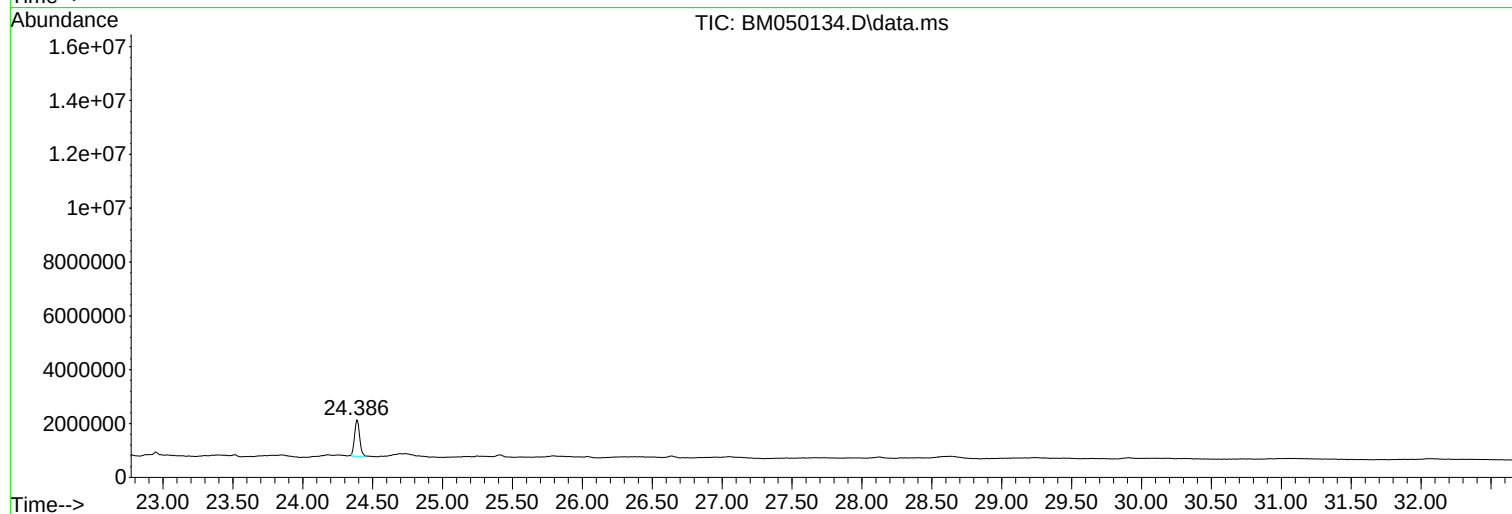
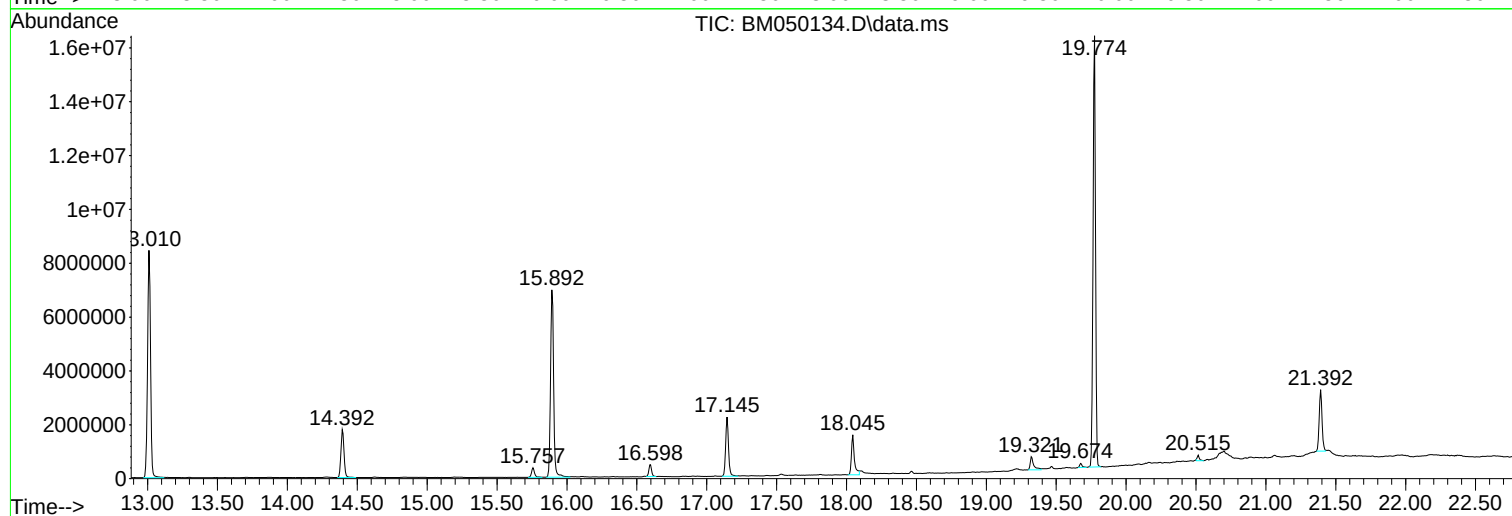
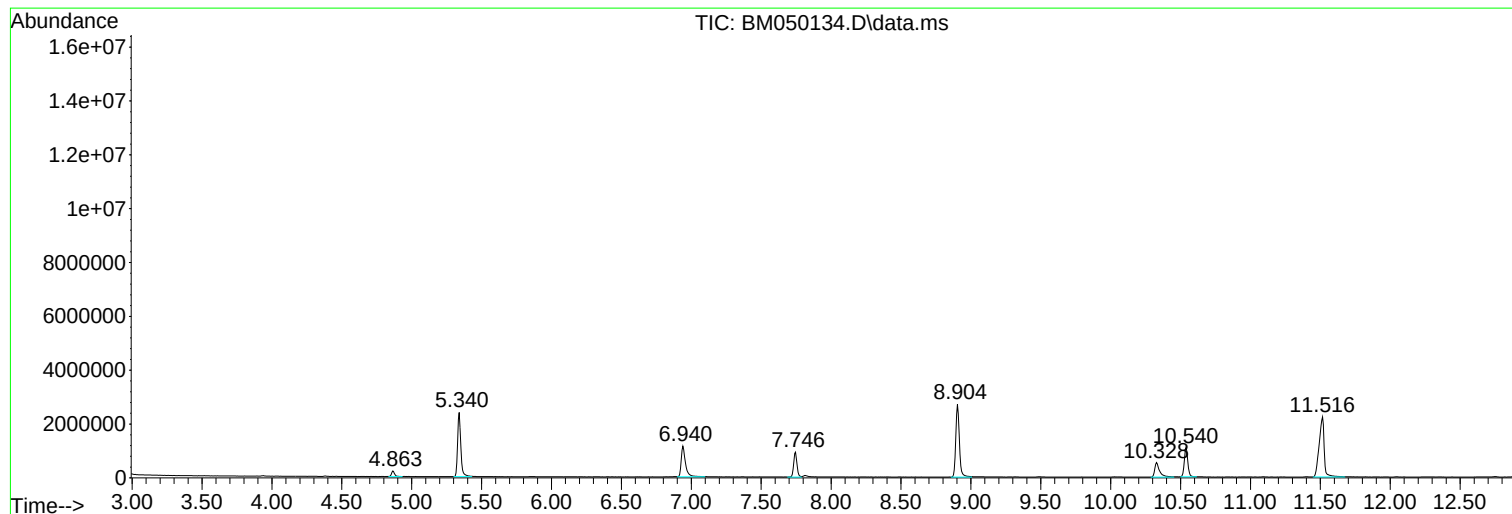
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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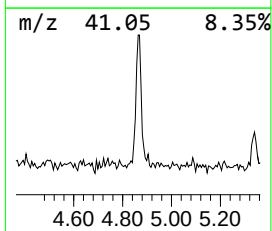
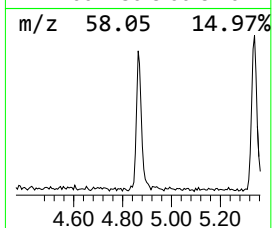
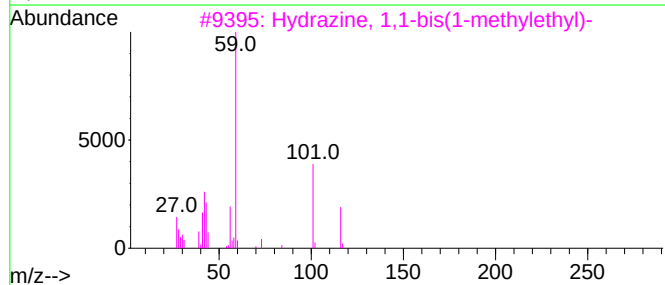
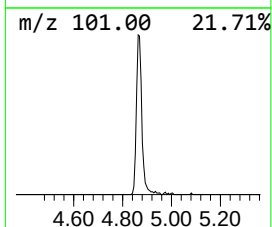
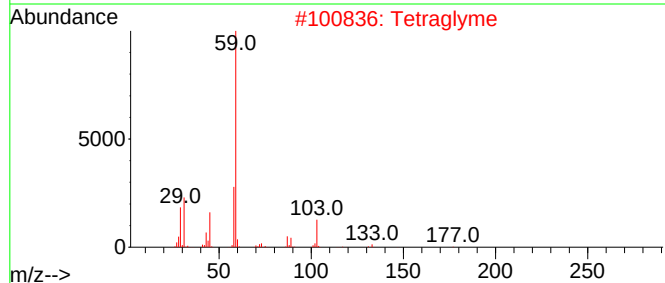
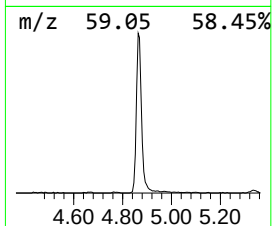
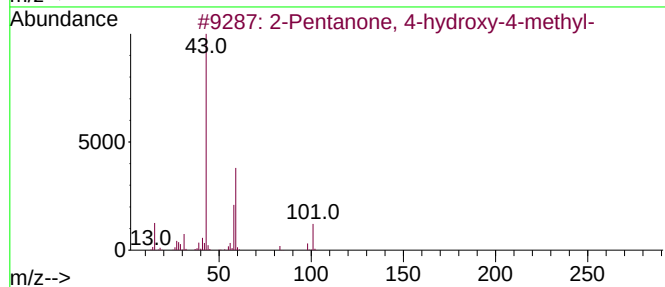
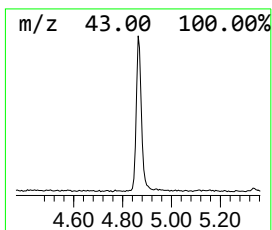
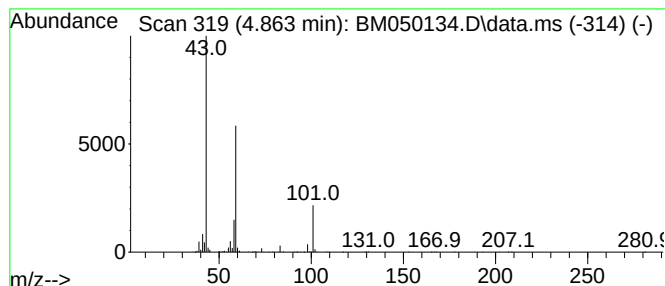
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.863	4.13 ng	310157	1,4-Dichlorobenzene-d4	7.746

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	Tetraglyme	222	C10H22O5	000143-24-8	37	
3	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28	
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	17	



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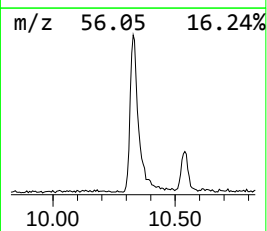
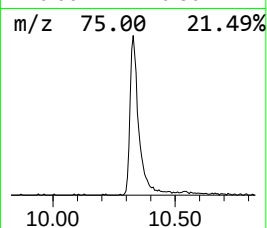
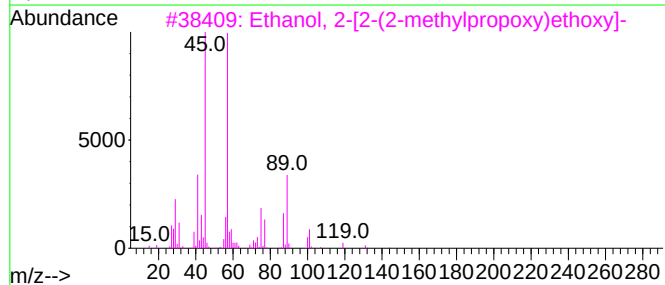
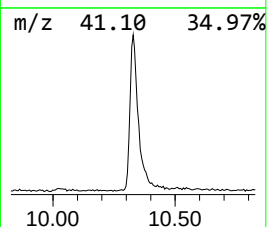
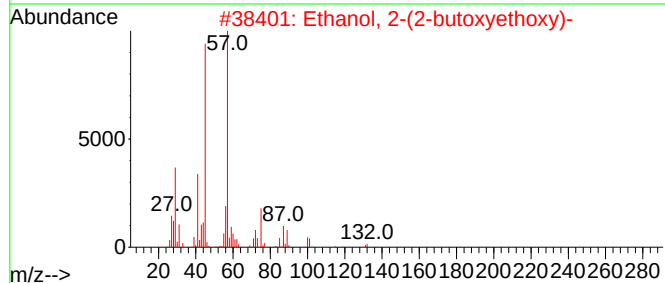
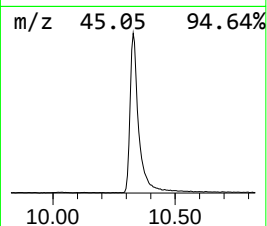
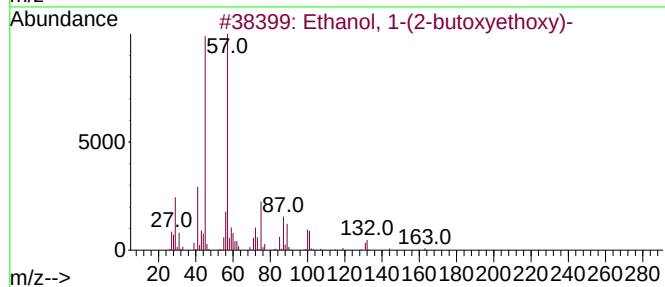
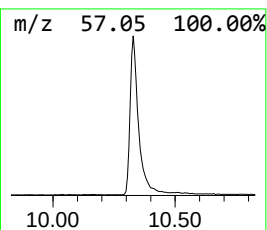
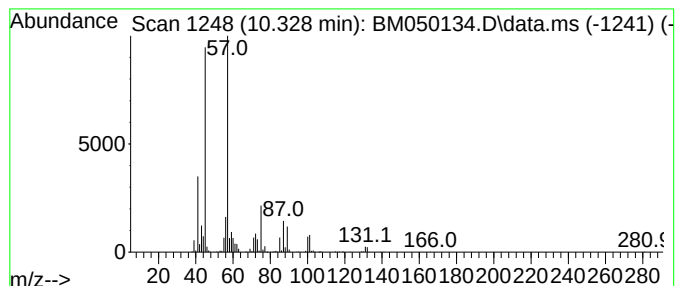
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Peak Number 2 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.328	13.69 ng	1312820	Naphthalene-d8	10.540

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3			Ethanol, 2-[2-(2-methylpropoxy)ethoxy]-	162	C8H18O3	018912-80-6	72
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	52
5			Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	50



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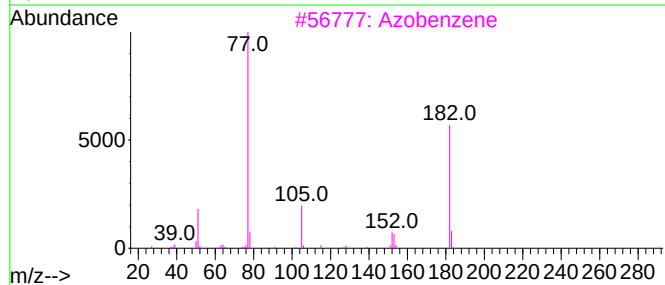
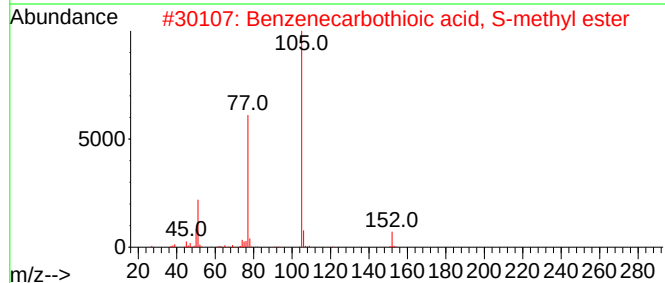
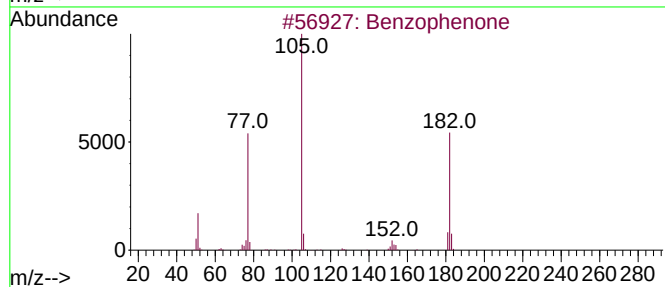
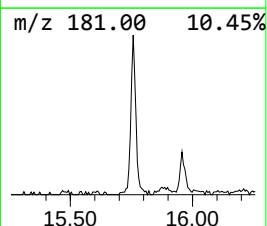
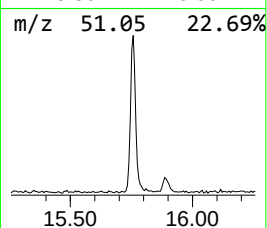
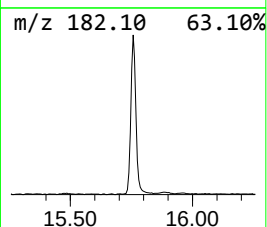
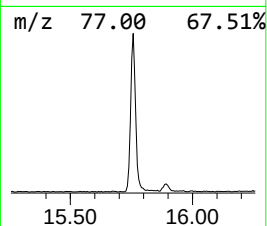
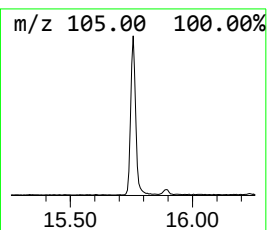
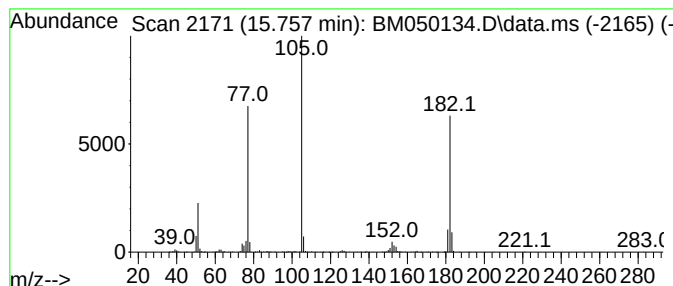
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Peak Number 3 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.757	3.79 ng	520261	Acenaphthene-d10	14.392

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	47
3			Azobenzene	182	C12H10N2	000103-33-3	47
4			N-[2,2-Dichloro-1-(toluene-4-sul...	371	C16H15Cl2NO3S	136800-77-6	43
5			Vinyl benzoate	148	C9H8O2	000769-78-8	43



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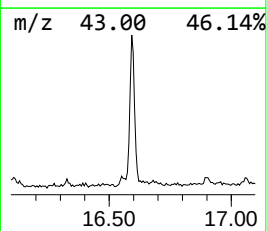
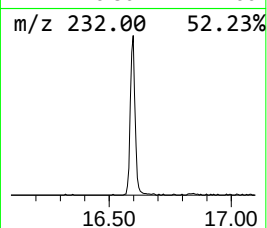
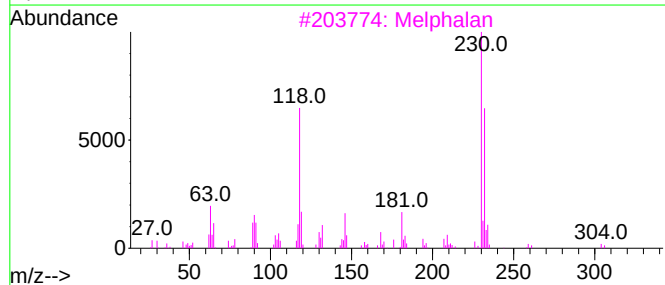
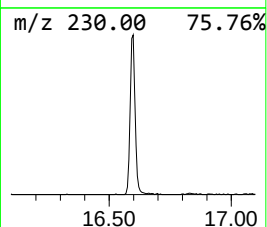
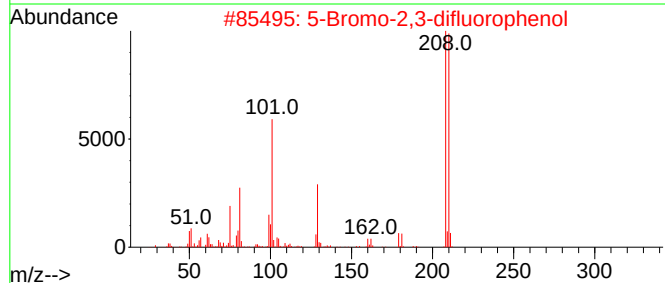
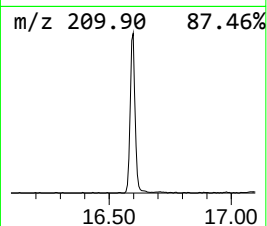
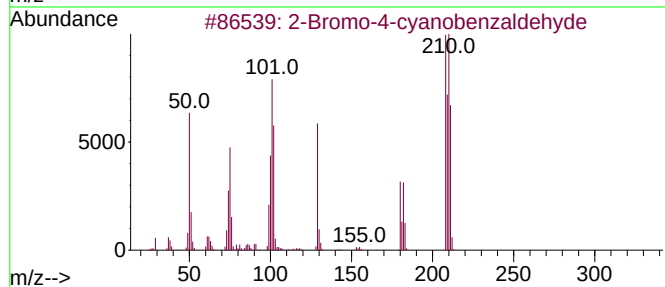
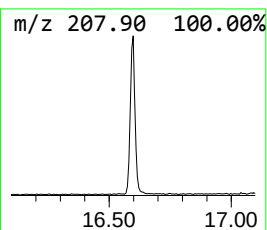
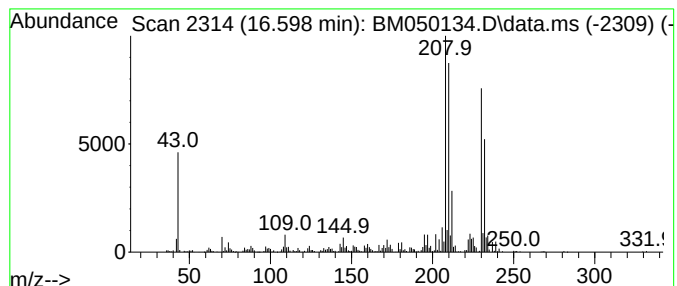
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Peak Number 4 unknown16.598 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.598	3.89 ng	616059	Phenanthrene-d10	17.145

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Bromo-4-cyanobenzaldehyde	209	C8H4BrNO	089891-69-0	38
2		5-Bromo-2,3-difluorophenol	208	C6H3BrF2O	186590-26-1	35
3		Melphalan	304	C13H18Cl2N2O2	000148-82-3	27
4		Methyl 2-amino-3-(4-(N,N-bis(2-c...	318	C14H20Cl2N2O2	1000468-61-4	22
5		2-(1-Piperazinyl)nicotinamide, N...	278	C13H22N4OSi	1000476-27-4	18



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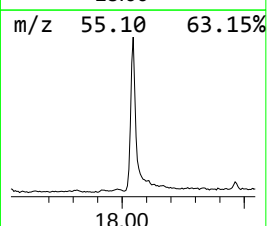
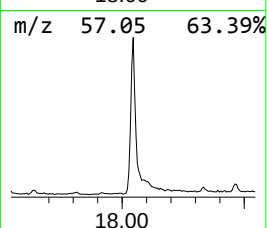
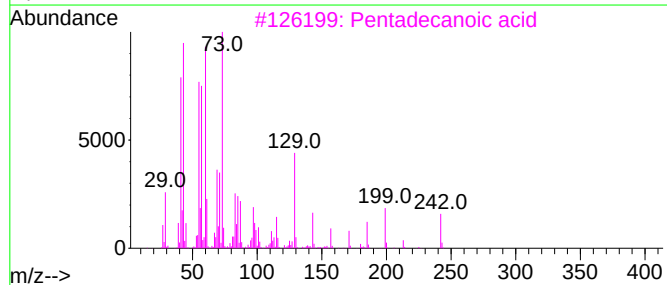
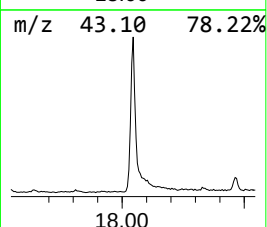
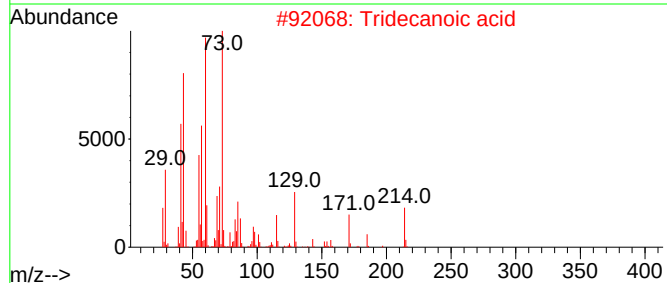
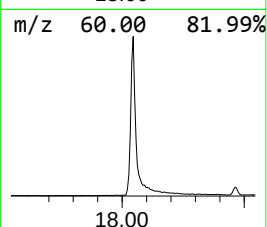
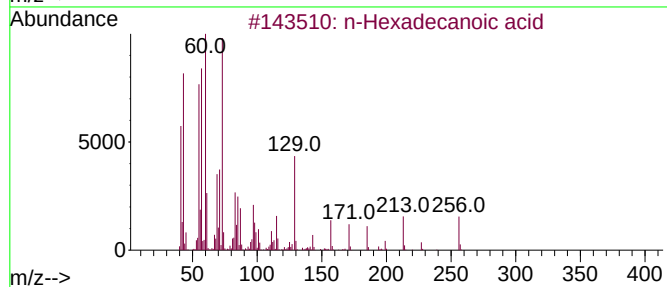
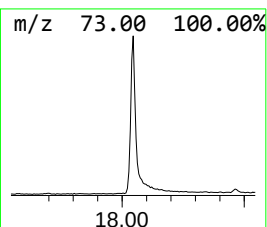
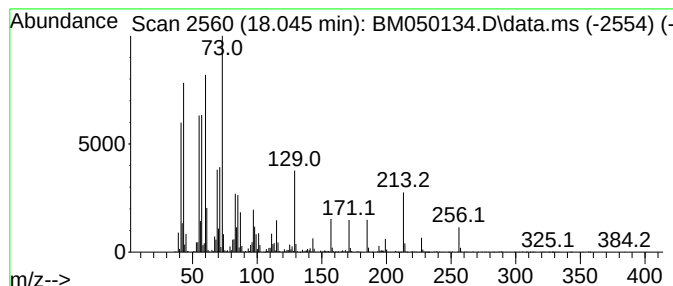
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.045	13.97 ng	2215520	Phenanthrene-d10	17.145

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	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Octadecanoic acid	284	C18H36O2	000057-11-4	87
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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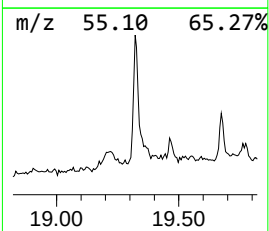
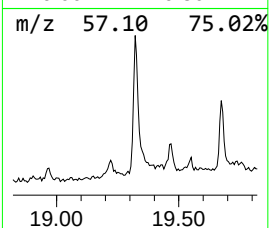
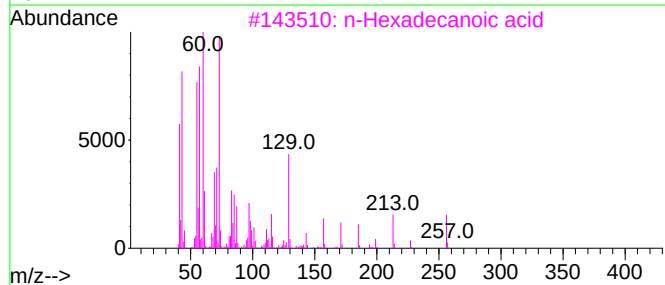
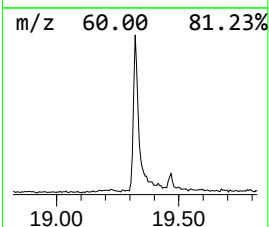
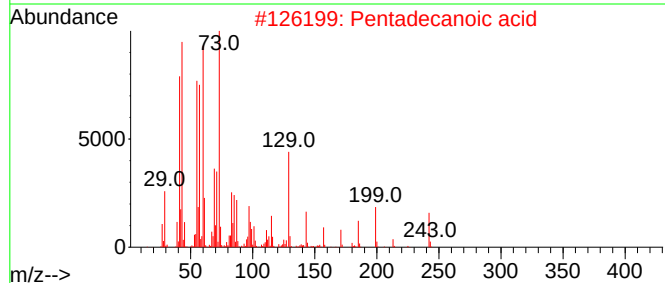
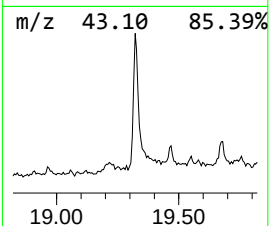
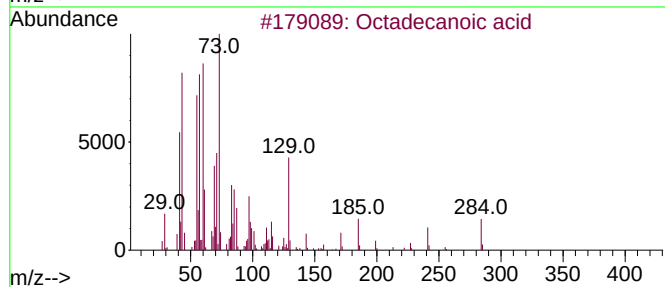
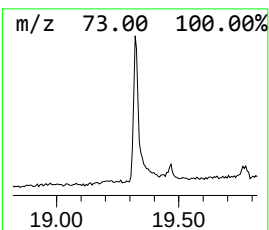
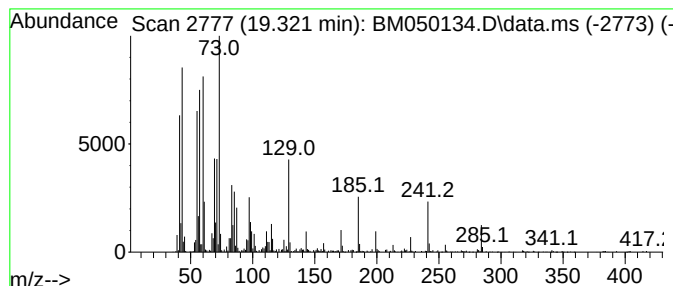
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.321	5.14 ng	839837	Chrysene-d12	21.392

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	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Tridecanoic acid	214	C13H26O2	000638-53-9	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM050725\
Data File : BM050134.D
Acq On : 07 May 2025 14:26
Operator : RC/JU
Sample : Q1945-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
GB1W

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042825.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
2-Pentanone, 4-...	4.863	4.1	ng	310157	1	7.746	1502810	20.0
Ethanol, 1-(2-b...	10.328	13.7	ng	1312820	2	10.540	1918340	20.0
Benzophenone	15.757	3.8	ng	520261	3	14.392	2743700	20.0
unknown16.598	16.598	3.9	ng	616059	4	17.145	3170700	20.0
n-Hexadecanoic ...	18.045	14.0	ng	2215520	4	17.145	3170700	20.0
Octadecanoic acid	19.321	5.1	ng	839837	5	21.392	3267110	20.0