

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041525\
 Data File : BM049931.D
 Acq On : 15 Apr 2025 12:37
 Operator : RC/JU
 Sample : Q1781-09
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 WC-11

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-BM040825.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM049931.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.893	318	324	331	rVB	288817	412048	1.76%	0.395%
2	5.357	397	403	421	rBV	3735171	5475403	23.41%	5.251%
3	5.963	501	506	516	rVB	197953	306777	1.31%	0.294%
4	6.951	666	674	687	rBV	3300331	5337681	22.82%	5.119%
5	7.769	805	813	822	rBV	1507553	2273886	9.72%	2.181%
6	8.928	1000	1010	1023	rBV	2038500	3338433	14.27%	3.202%
7	10.563	1281	1288	1302	rBV	1613280	2751832	11.76%	2.639%
8	13.033	1701	1708	1723	rBV	5594055	7871997	33.65%	7.550%
9	14.416	1936	1943	1958	rBV	2462992	3598289	15.38%	3.451%
10	15.774	2168	2174	2182	rBV	440026	626262	2.68%	0.601%
11	15.904	2190	2196	2215	rBV	4836503	6781538	28.99%	6.504%
12	17.157	2403	2409	2423	rVB2	2555826	3755285	16.05%	3.602%
13	17.833	2520	2524	2530	rBV	183830	245376	1.05%	0.235%
14	18.074	2554	2565	2612	rBV	8608068	20107525	85.96%	19.284%
15	19.145	2743	2747	2751	rBV	457246	562307	2.40%	0.539%
16	19.221	2752	2760	2768	rBV5	375062	1237163	5.29%	1.187%
17	19.350	2773	2782	2818	rVV	11351571	23391092	100.00%	22.433%
18	19.786	2851	2856	2863	rVB	7454900	8600834	36.77%	8.249%
19	21.397	3125	3130	3144	rVB	2536568	3671481	15.70%	3.521%
20	24.403	3634	3641	3652	rVB	1580886	3923392	16.77%	3.763%

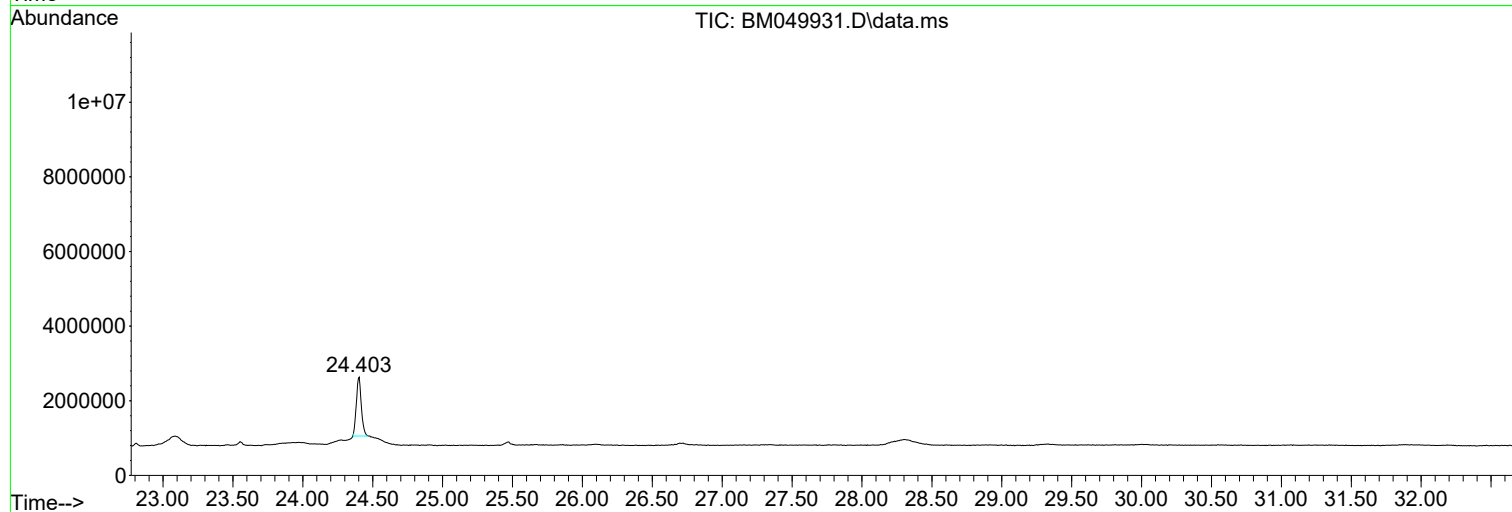
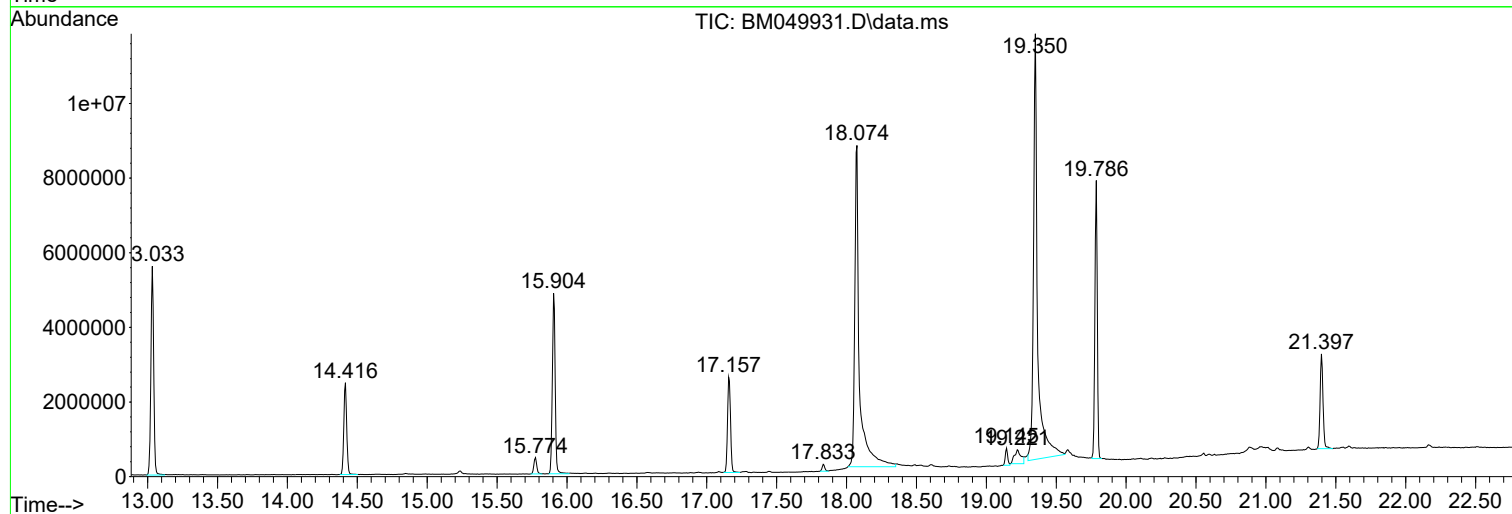
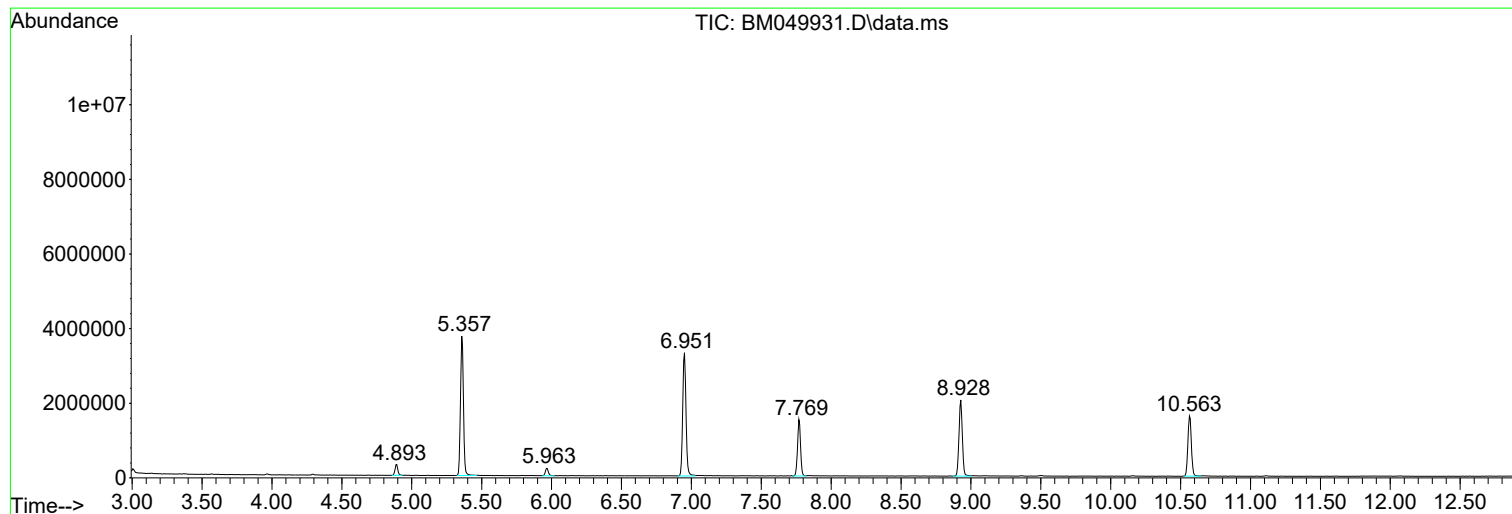
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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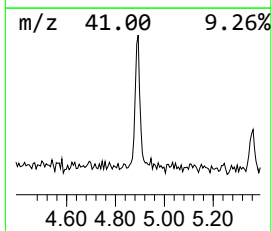
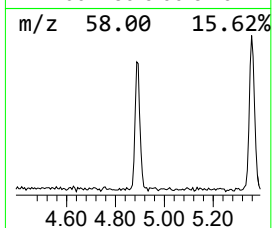
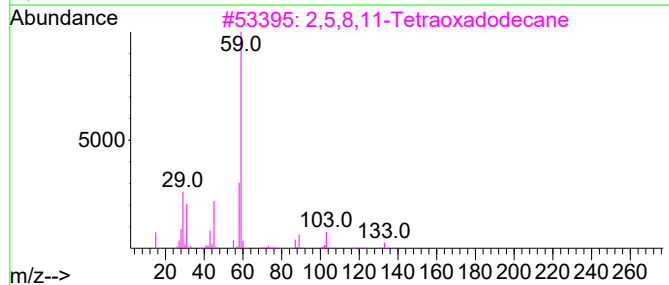
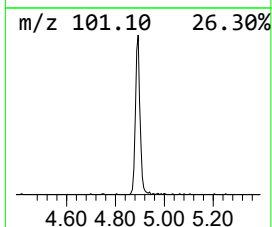
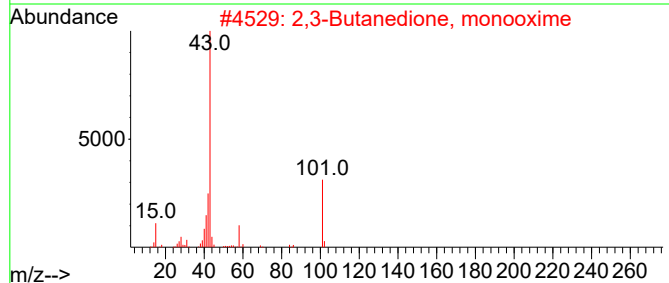
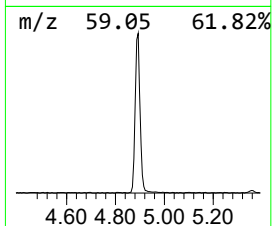
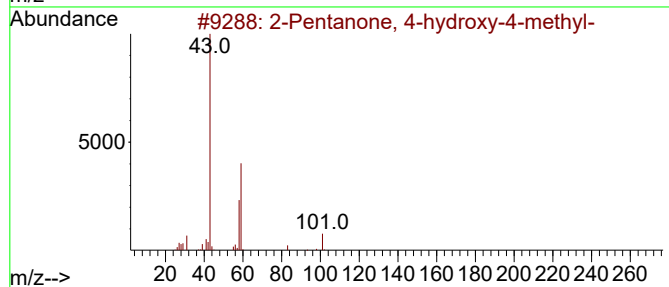
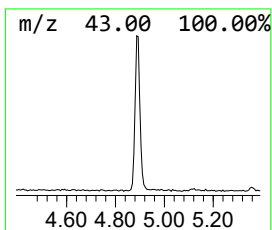
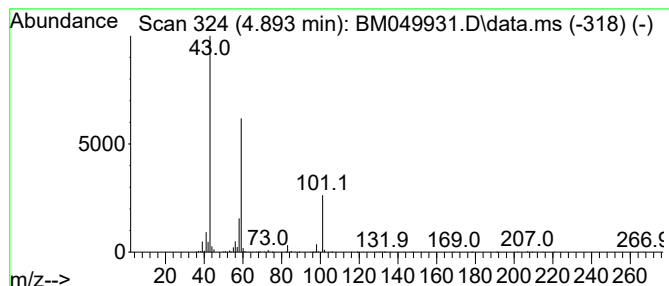
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.893	3.62 ng	412048	1,4-Dichlorobenzene-d4	7.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
3	2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	25		
4	Tetraglyme	222	C10H22O5	000143-24-8	23		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		



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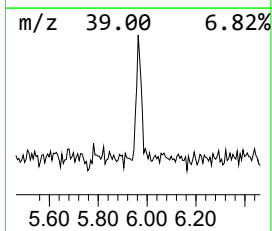
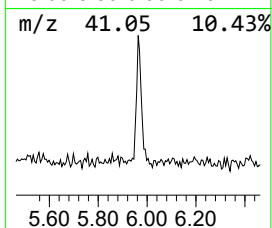
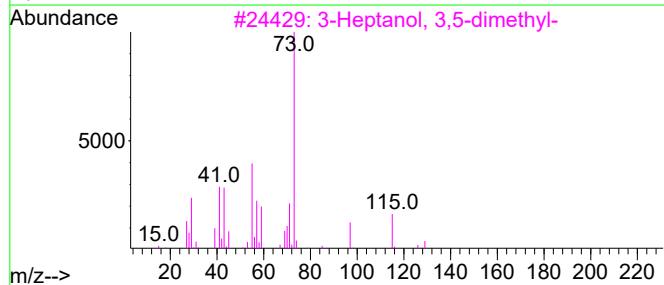
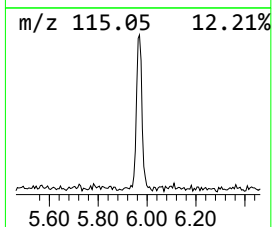
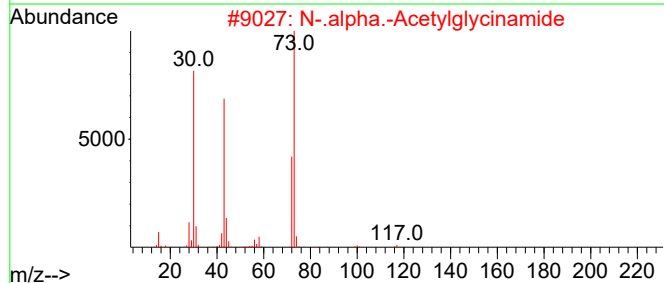
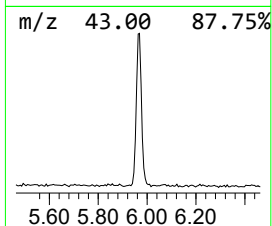
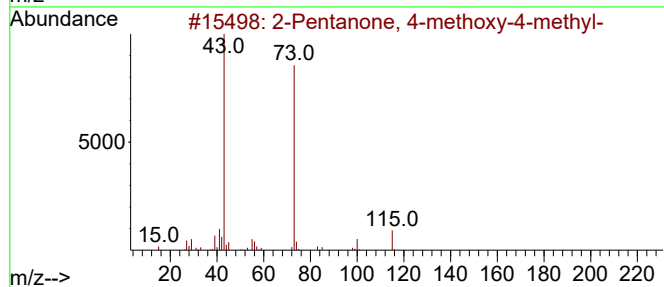
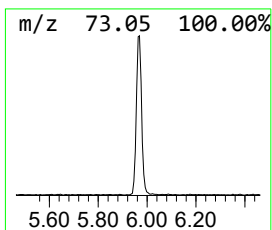
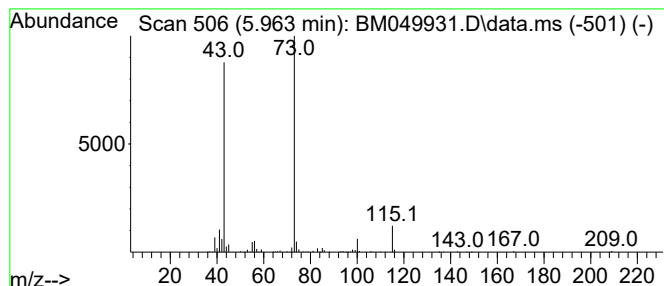
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.963	2.70 ng	306777	1,4-Dichlorobenzene-d4	7.769

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	28
3		3-Heptanol, 3,5-dimethyl-	144	C9H20O	019549-74-7	25
4		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	22
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	16



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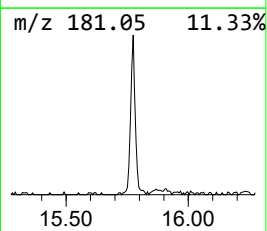
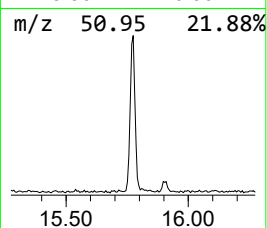
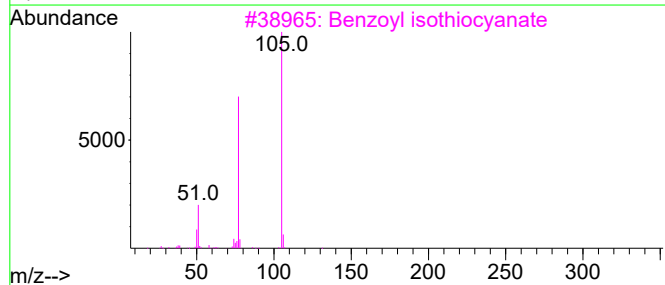
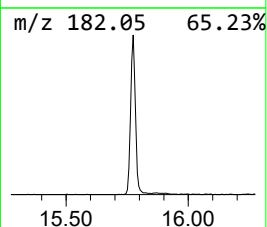
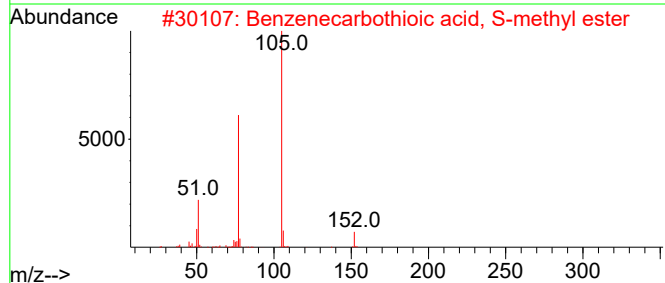
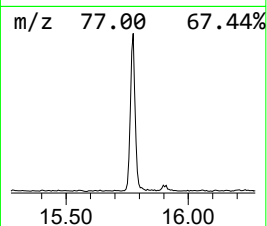
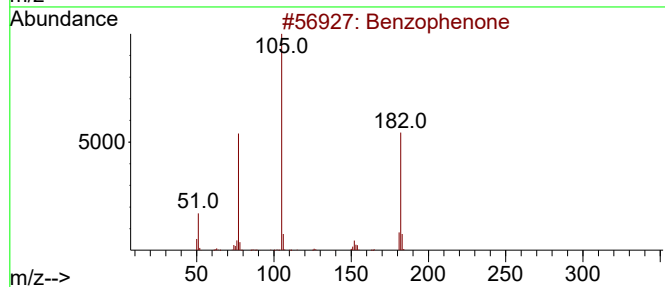
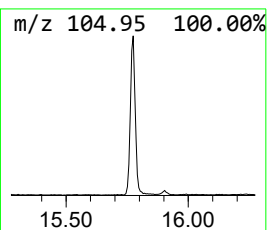
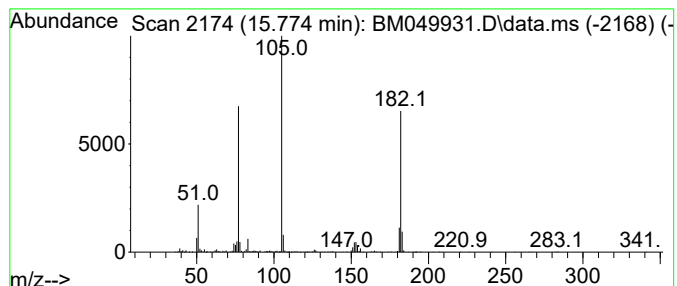
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.774	3.48 ng	626262	Acenaphthene-d10	14.416

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	43
3			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	38
4			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	38
5			Isopropyl phenyl ketone	148	C10H12O	000611-70-1	38



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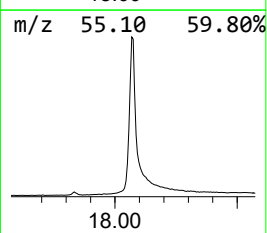
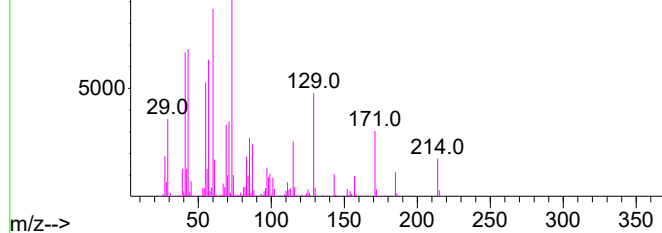
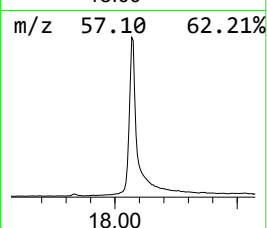
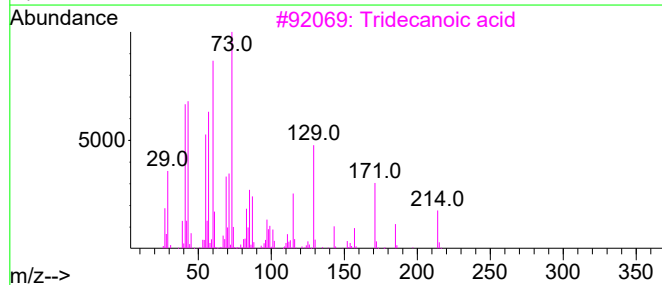
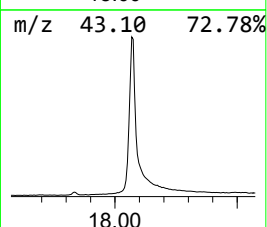
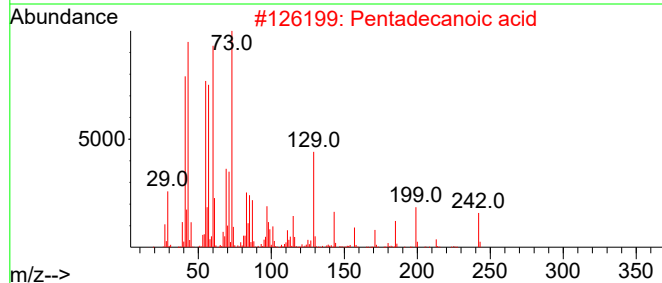
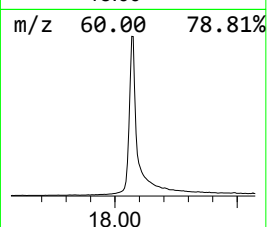
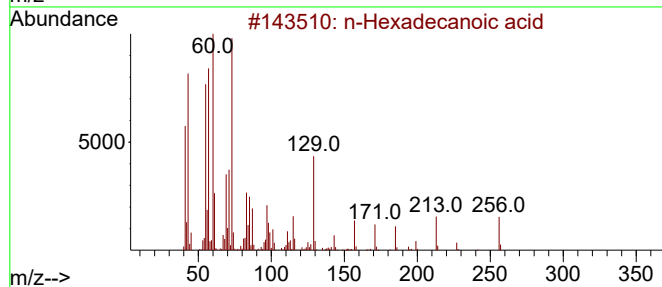
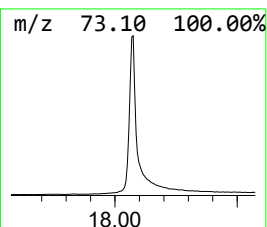
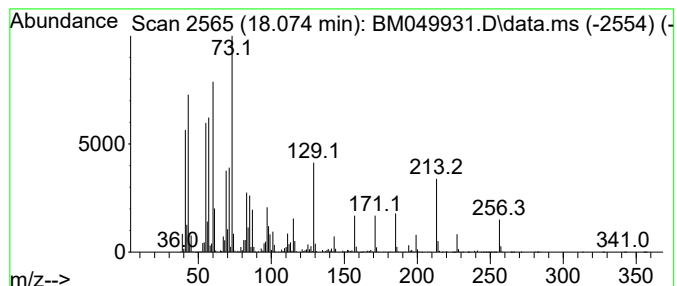
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.074	107.09 ng	20107500	Phenanthrene-d10	17.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	86
4			Undecanoic acid	186	C11H22O2	000112-37-8	83
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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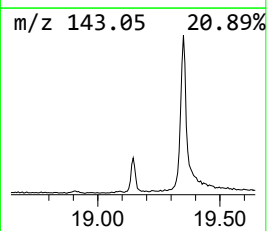
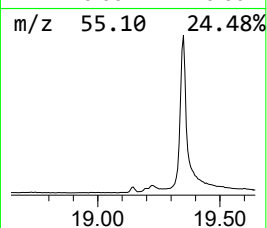
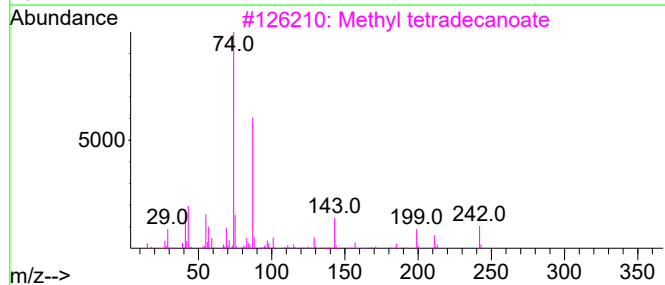
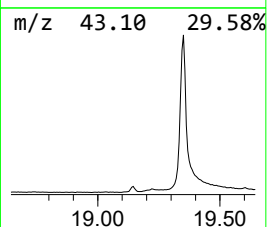
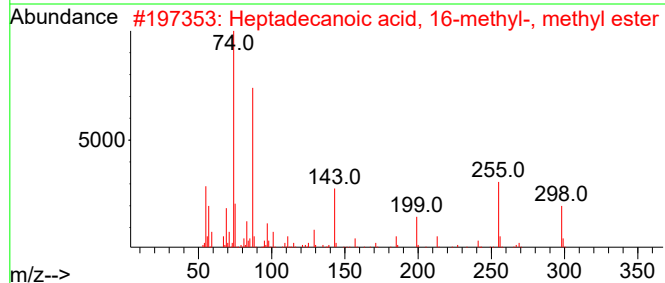
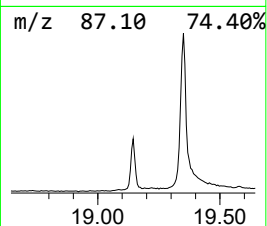
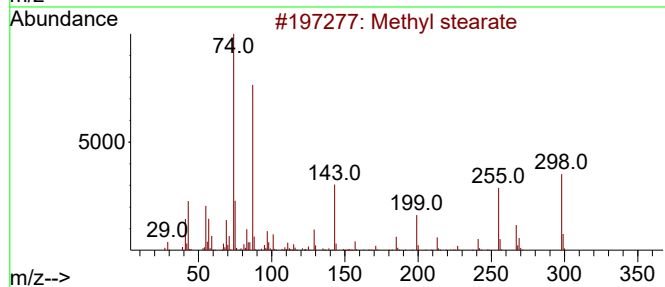
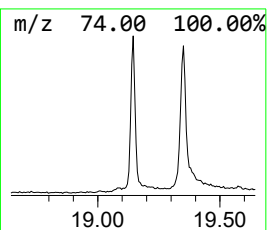
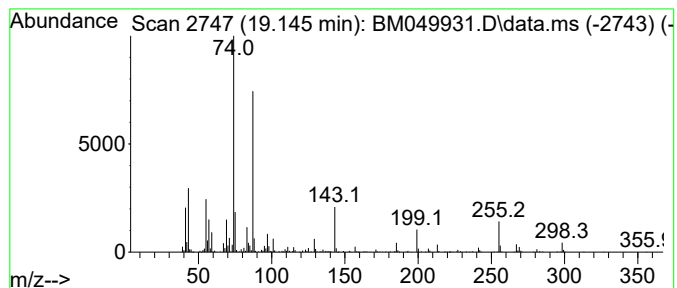
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Peak Number 5 Methyl stearate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.145	2.99 ng	562307	Phenanthrene-d10	17.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	98
2			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	89
3			Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
4			2-Methylpentadecanoic acid	256	C16H32O2	025354-92-1	83
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	83



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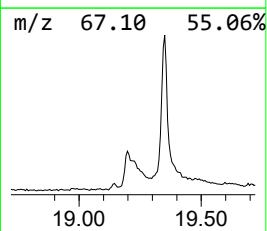
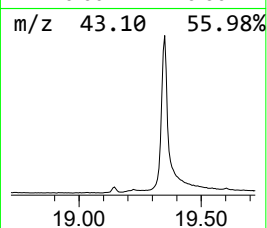
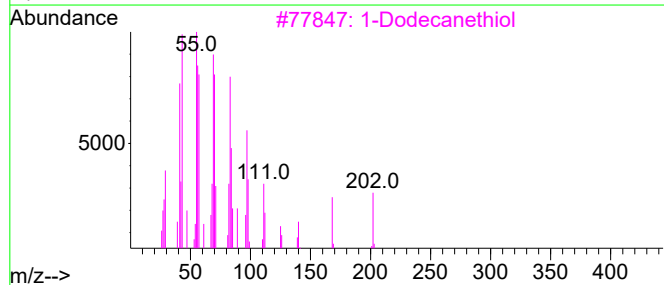
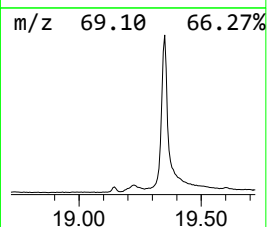
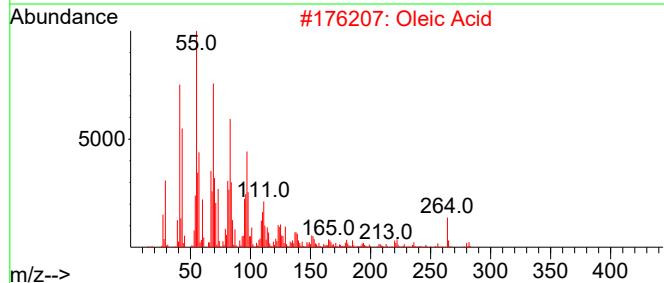
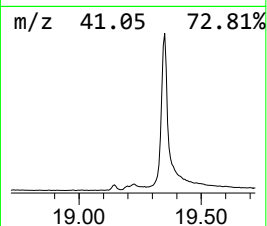
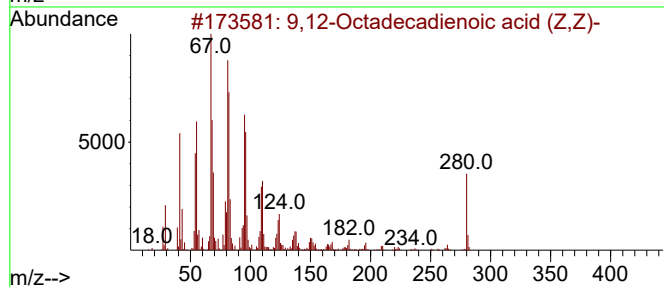
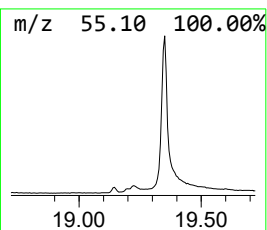
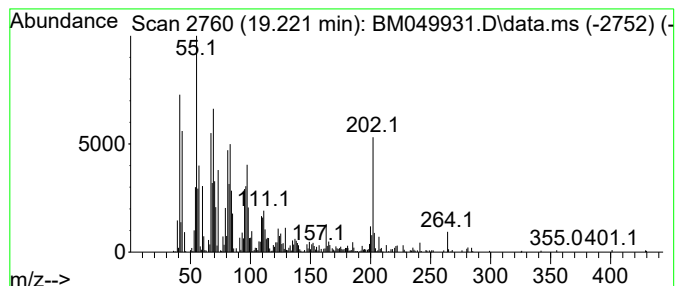
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9,12-Octadecadienoic acid (... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.221	6.59 ng	1237160	Phenanthrene-d10	17.157

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	90
2		Oleic Acid	282	C18H34O2	000112-80-1	70
3		1-Dodecanethiol	202	C12H26S	000112-55-0	68
4		cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	68
5		9-Eicosenoic acid, (Z)-	310	C20H38O2	029204-02-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041525\
Data File : BM049931.D
Acq On : 15 Apr 2025 12:37
Operator : RC/JU
Sample : Q1781-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

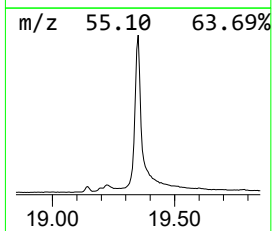
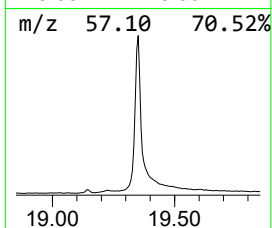
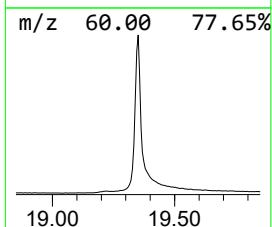
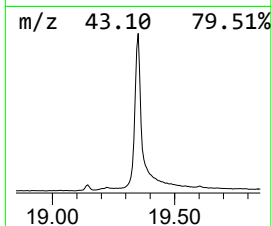
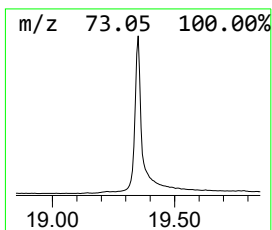
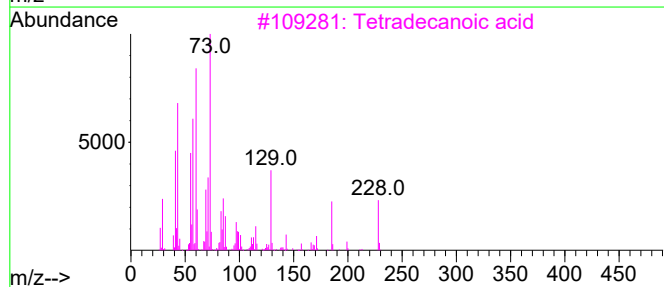
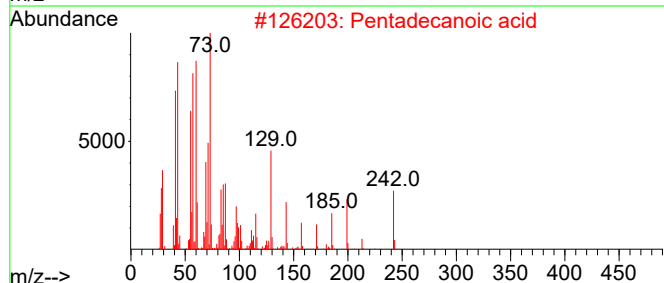
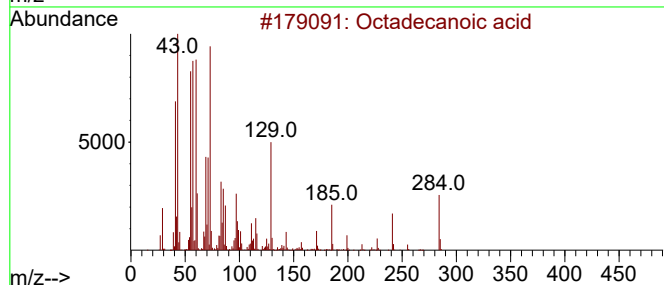
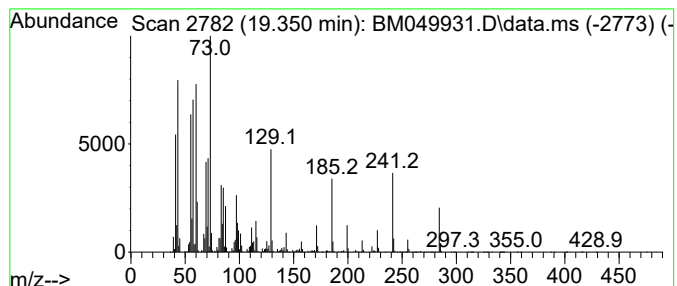
Instrument :
BNA_M
ClientSampleId :
WC-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.351	127.42 ng	23391100	Chrysene-d12	21.397	
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	74
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041525\
Data File : BM049931.D
Acq On : 15 Apr 2025 12:37
Operator : RC/JU
Sample : Q1781-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.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-...	4.893	3.6	ng	412048	1	7.769	2273890	20.0
2-Pentanone, 4-...	5.963	2.7	ng	306777	1	7.769	2273890	20.0
Benzophenone	15.774	3.5	ng	626262	3	14.416	3598290	20.0
n-Hexadecanoic ...	18.074	107.1	ng	20107500	4	17.157	3755290	20.0
Methyl stearate	19.145	3.0	ng	562307	4	17.157	3755290	20.0
9,12-Octadecadi...	19.221	6.6	ng	1237160	4	17.157	3755290	20.0
Octadecanoic acid	19.351	127.4	ng	23391100	5	21.397	3671480	20.0