

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM050925\
 Data File : BM050160.D
 Acq On : 09 May 2025 15:27
 Operator : RC/JU
 Sample : Q1986-07
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 COMP-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-BM042825.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM050160.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	313	319	327	rBV	364090	532587	4.36%	0.751%
2	5.334	393	399	417	rBV	3497959	5639402	46.17%	7.956%
3	6.934	664	671	701	rBV	3077874	6098811	49.93%	8.604%
4	7.739	801	808	819	rBV	1204569	1955564	16.01%	2.759%
5	8.904	998	1006	1030	rBV	1825934	3715079	30.42%	5.241%
6	10.533	1276	1283	1305	rBV	1267202	2607751	21.35%	3.679%
7	13.004	1696	1703	1730	rBV	5507765	8918924	73.02%	12.582%
8	14.392	1931	1939	1956	rBV	2374098	3828258	31.34%	5.401%
9	15.751	2163	2170	2183	rBV	698723	1120911	9.18%	1.581%
10	15.892	2187	2194	2219	rVV	5192997	8635942	70.70%	12.183%
11	17.145	2400	2407	2422	rBV	2730174	4332278	35.47%	6.112%
12	18.039	2553	2559	2576	rBV	1610753	2756058	22.56%	3.888%
13	18.903	2699	2706	2713	rBV2	258072	455666	3.73%	0.643%
14	19.321	2772	2777	2791	rBV	430137	894575	7.32%	1.262%
15	19.768	2847	2853	2865	rBV	10083324	12214092	100.00%	17.231%
16	20.056	2897	2902	2911	rBV2	162728	325627	2.67%	0.459%
17	20.409	2959	2962	2967	rVB	125271	141570	1.16%	0.200%
18	21.056	3068	3072	3080	rVB2	398784	619013	5.07%	0.873%
19	21.386	3123	3128	3144	rVB	1917737	3226345	26.41%	4.552%
20	24.385	3630	3638	3657	rVB	976640	2865632	23.46%	4.043%

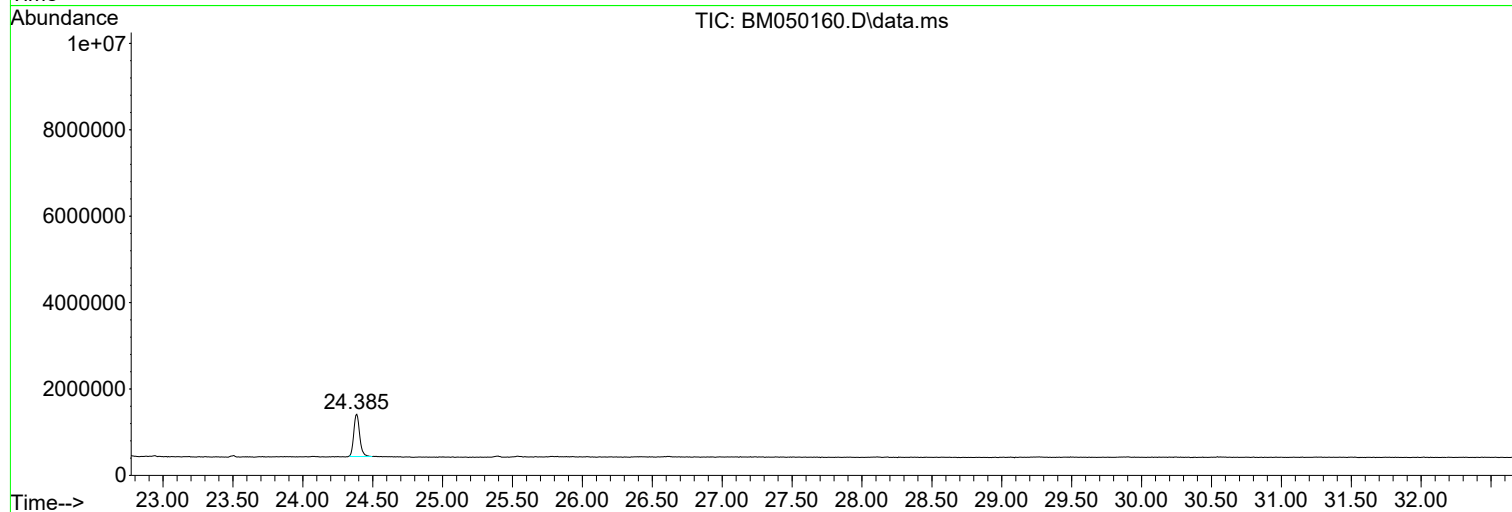
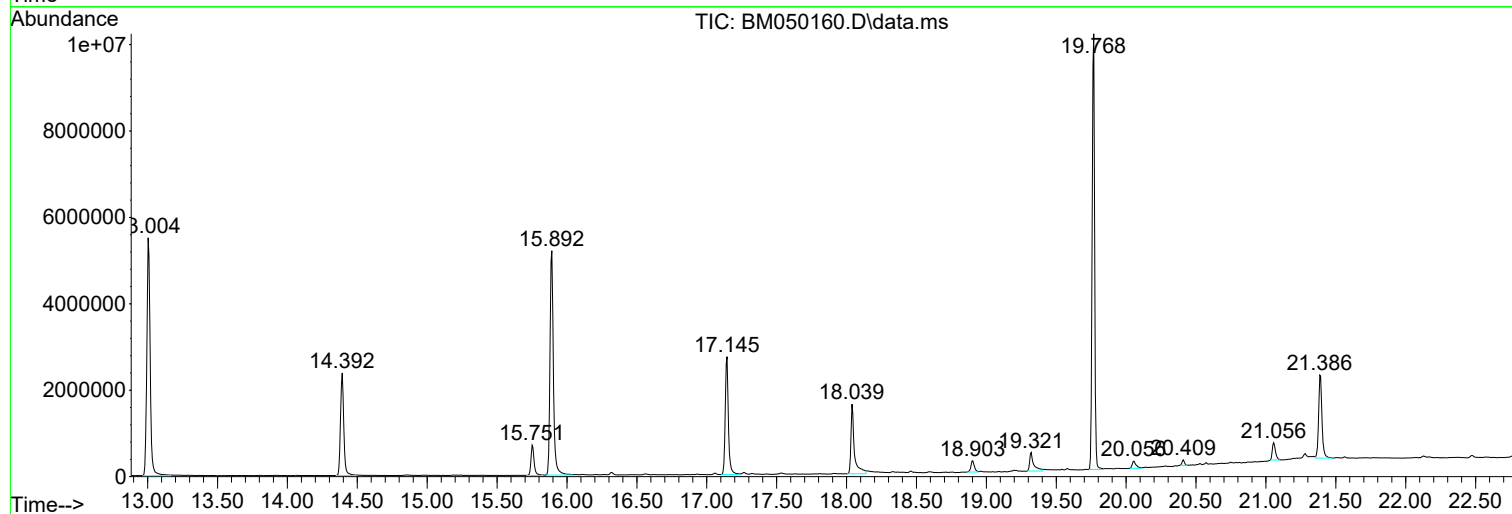
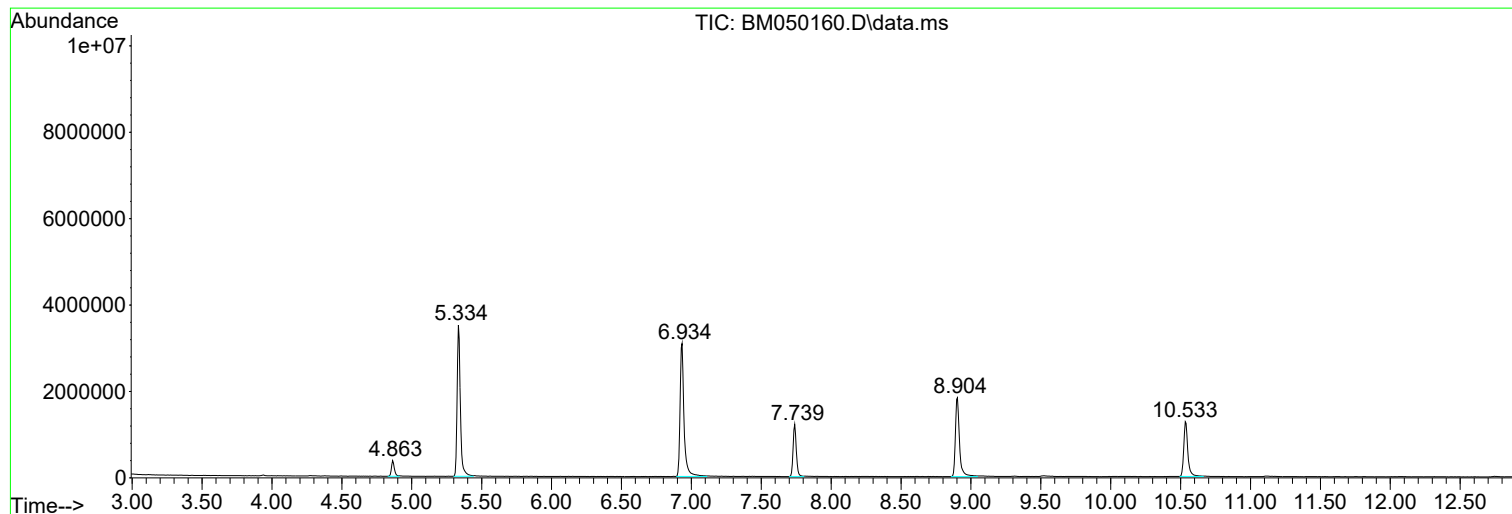
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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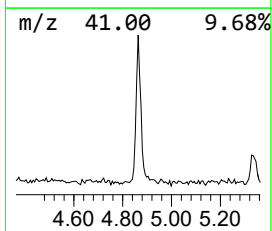
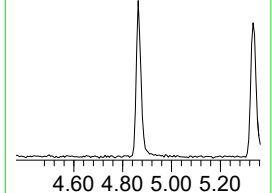
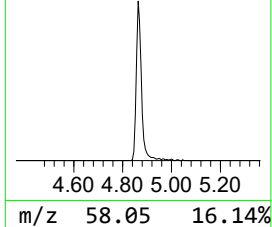
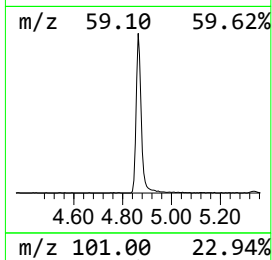
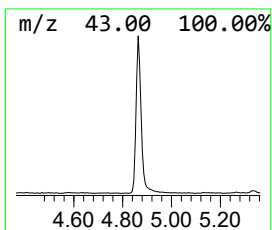
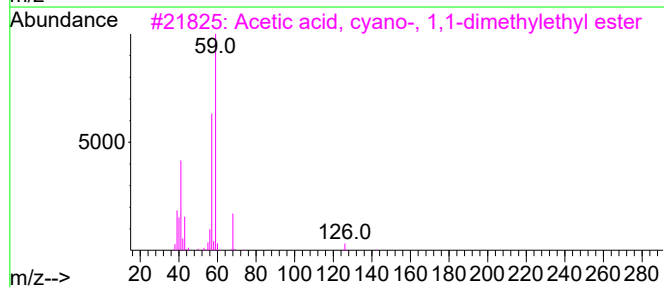
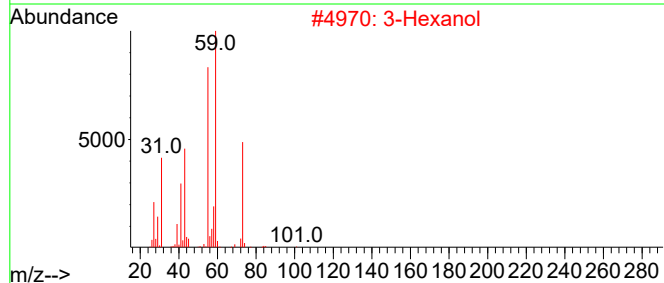
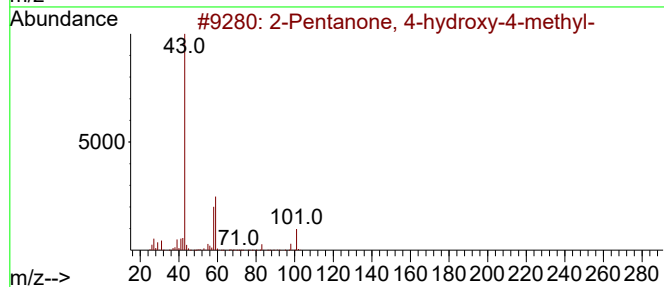
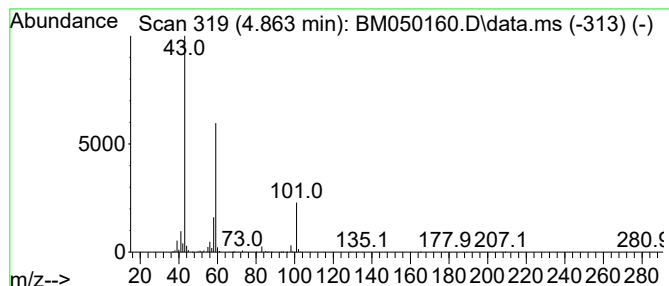
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	5.45 ng	532587	1,4-Dichlorobenzene-d4	7.739

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	3-Hexanol	102	C6H14O	000623-37-0	28		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	23		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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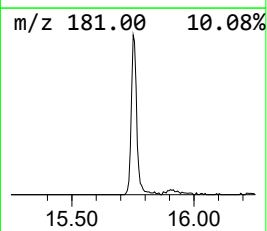
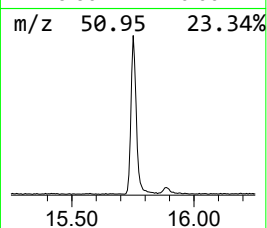
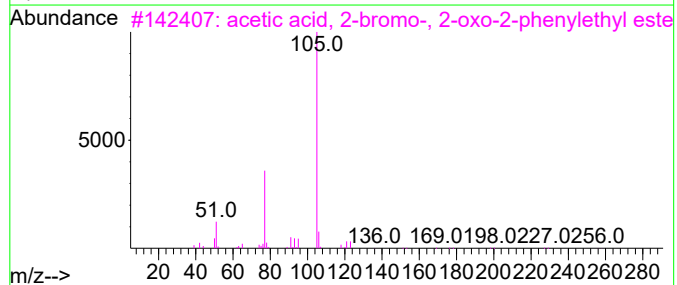
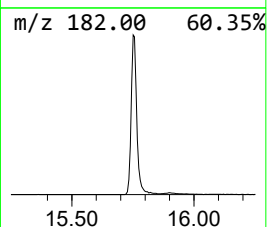
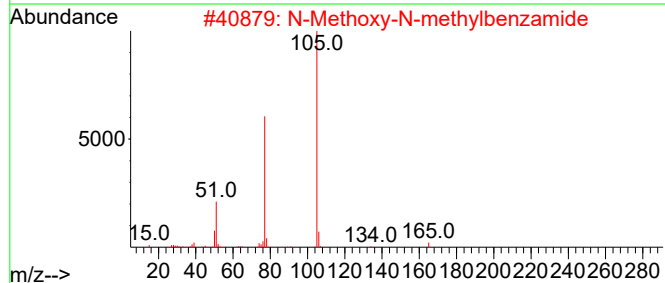
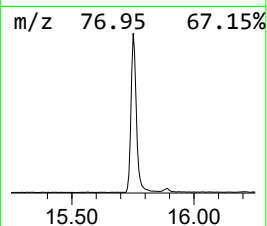
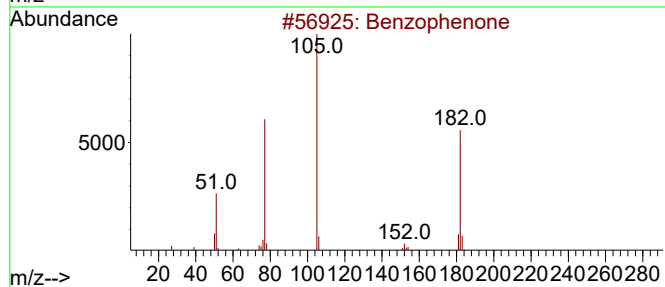
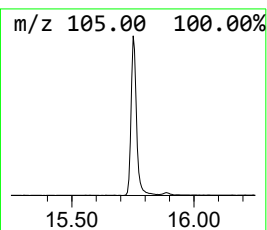
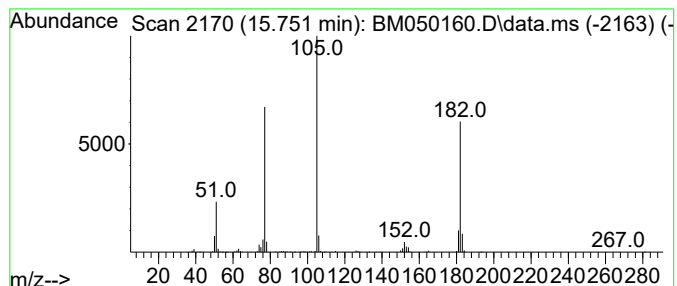
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.751	5.86 ng	1120910	Acenaphthene-d10	14.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	49
3			acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	47
4			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
5			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47



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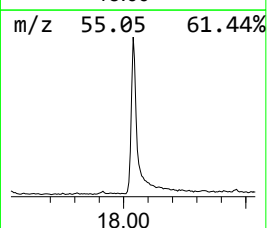
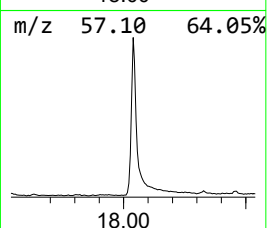
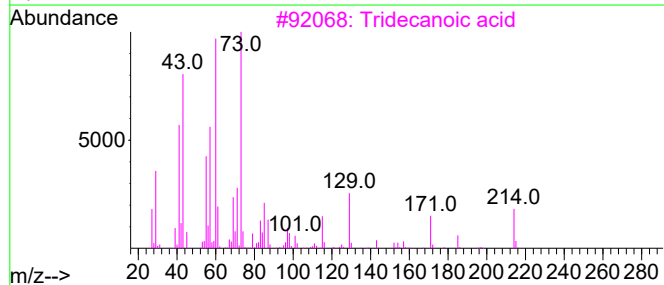
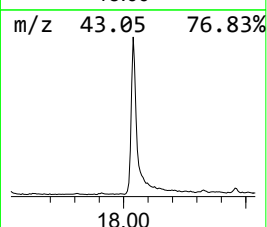
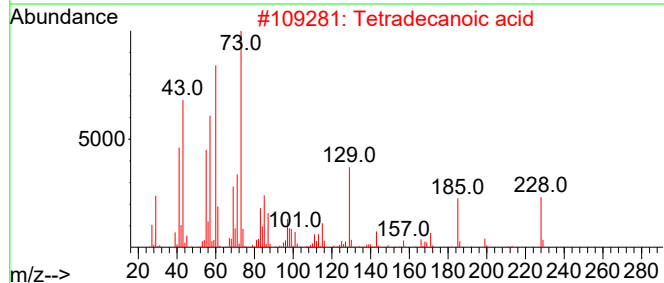
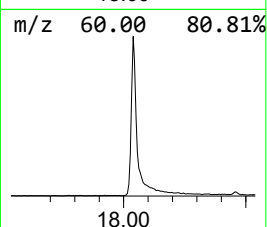
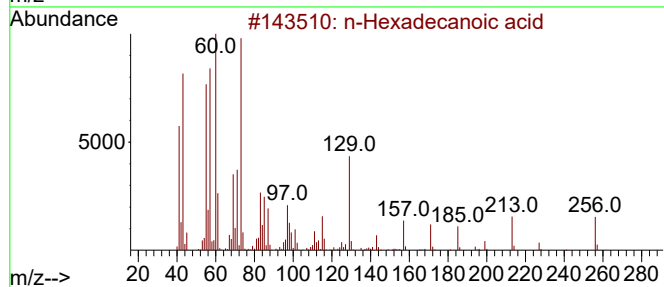
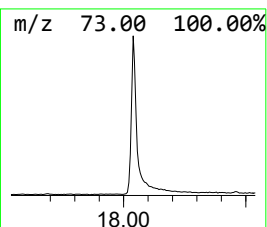
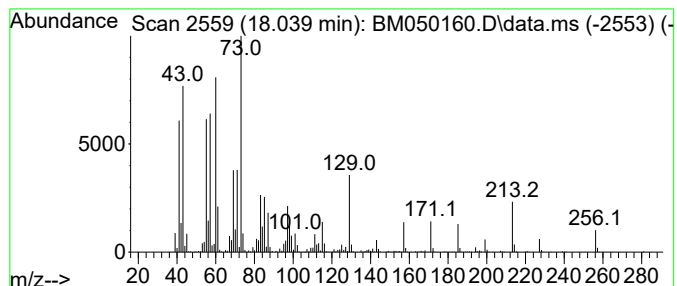
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.039	12.72 ng	2756060	Phenanthrene-d10	17.145

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	89
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Dodecanoic acid	200	C12H24O2	000143-07-7	52



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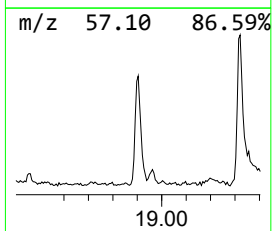
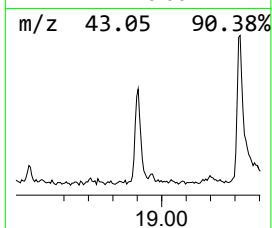
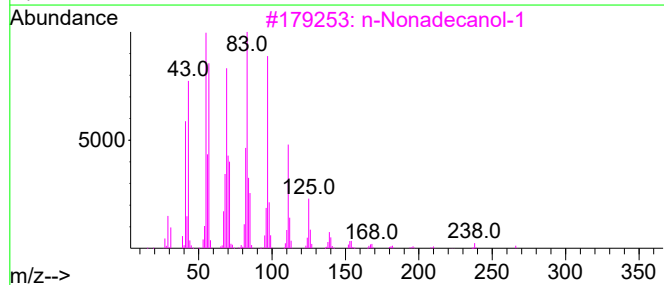
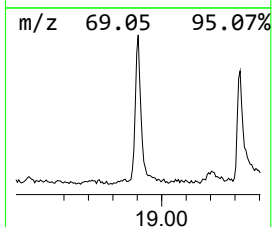
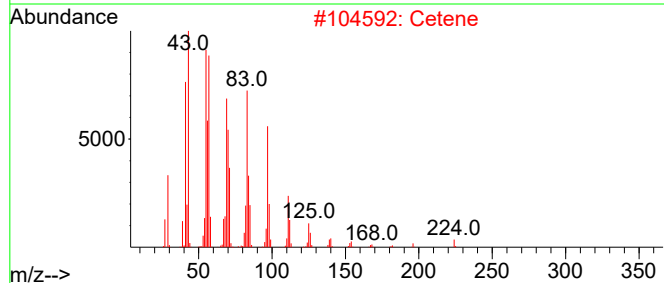
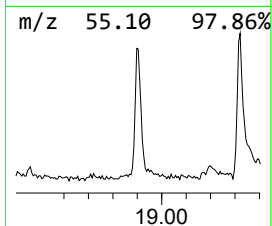
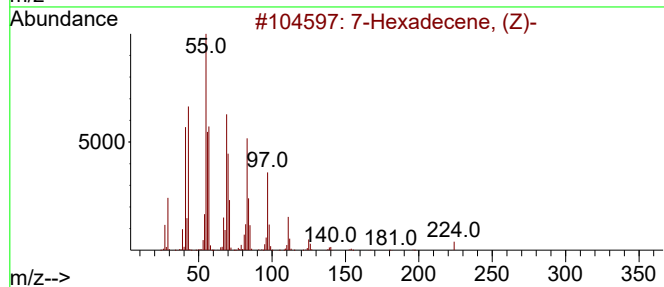
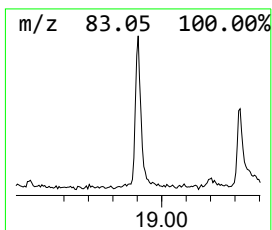
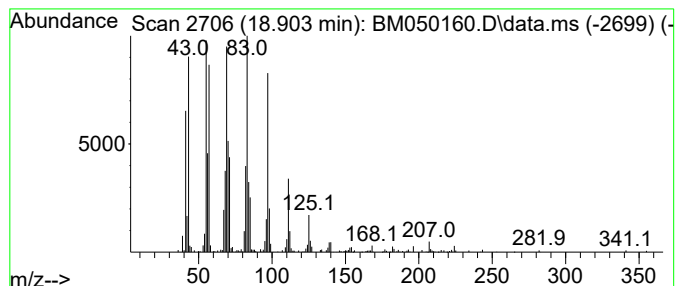
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 7-Hexadecene, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.904	2.10 ng	455666	Phenanthrene-d10		17.145	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	7-Hexadecene, (Z)-		224	C16H32	035507-09-6	95
2	Cetene		224	C16H32	000629-73-2	94
3	n-Nonadecanol-1		284	C19H40O	001454-84-8	91
4	1-Octadecanol		270	C18H38O	000112-92-5	91
5	3-Eicosene, (E)-		280	C20H40	074685-33-9	91



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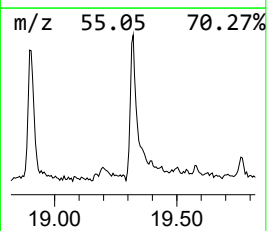
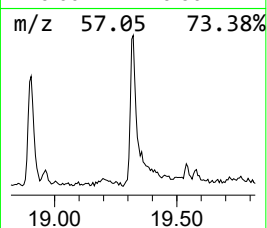
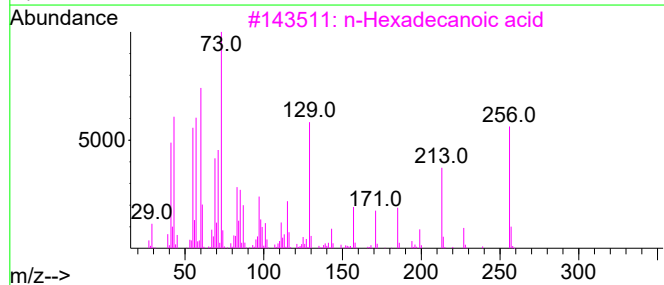
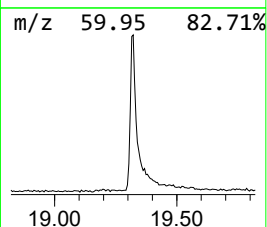
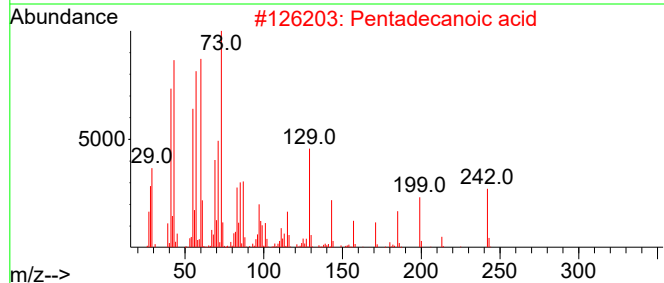
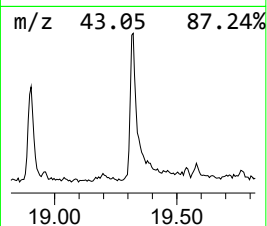
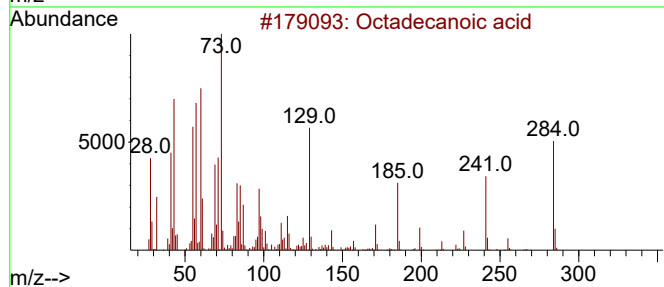
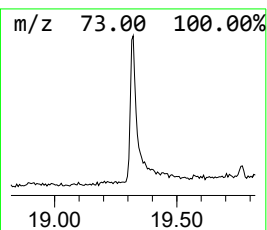
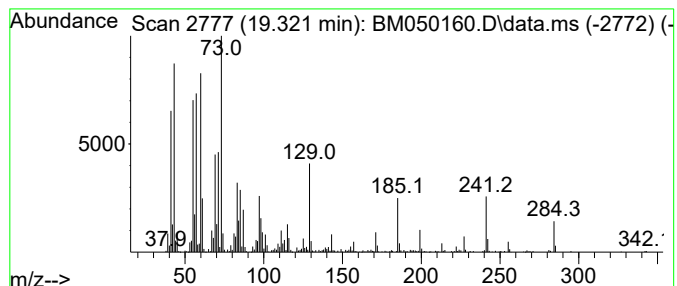
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Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.321	5.55 ng	894575	Chrysene-d12	21.386

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	91
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	83



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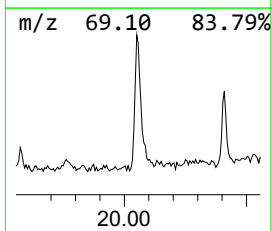
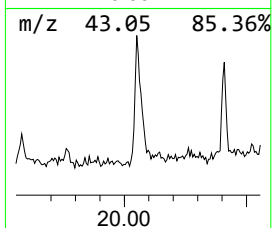
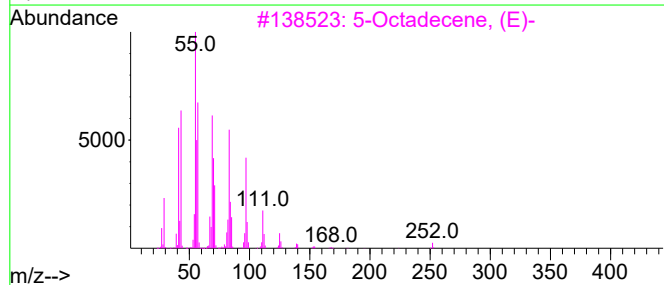
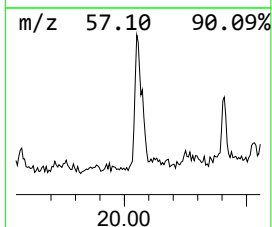
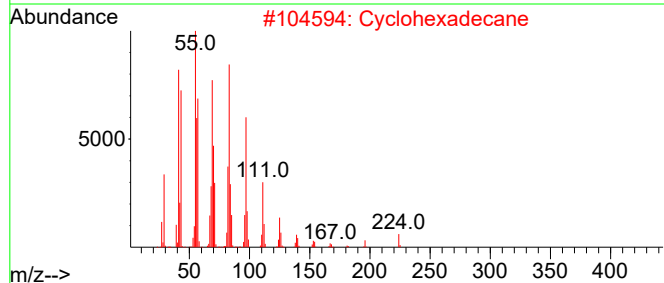
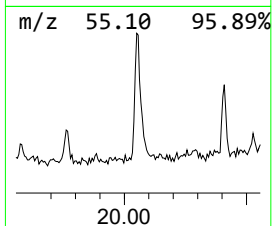
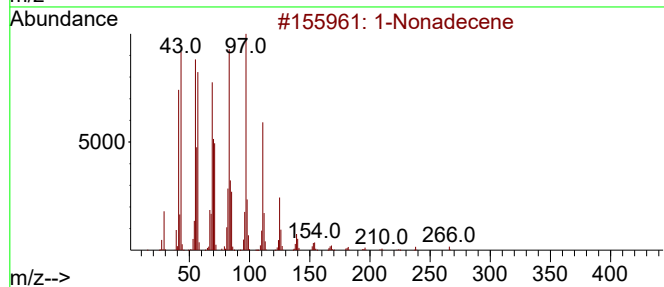
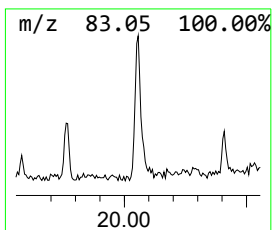
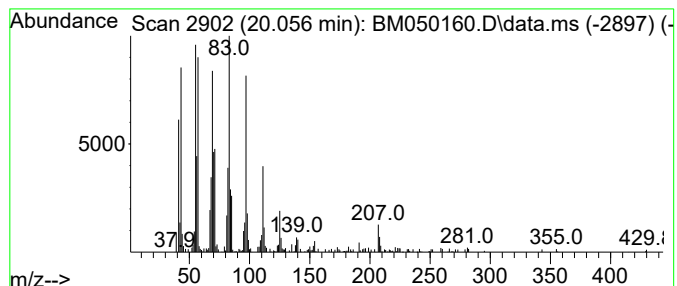
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Nonadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.056	2.02 ng	325627	Chrysene-d12	21.386

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Nonadecene	266	C19H38	018435-45-5	98
2		Cyclohexadecane	224	C16H32	000295-65-8	98
3		5-Octadecene, (E)-	252	C18H36	007206-21-5	97
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
5		1-Octadecanol	270	C18H38O	000112-92-5	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM050925\
Data File : BM050160.D
Acq On : 09 May 2025 15:27
Operator : RC/JU
Sample : Q1986-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-11

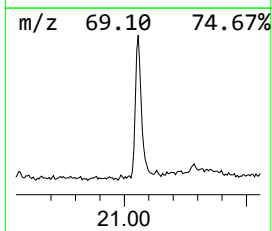
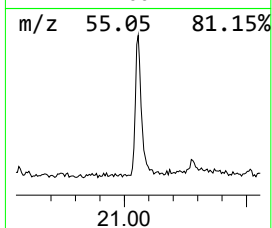
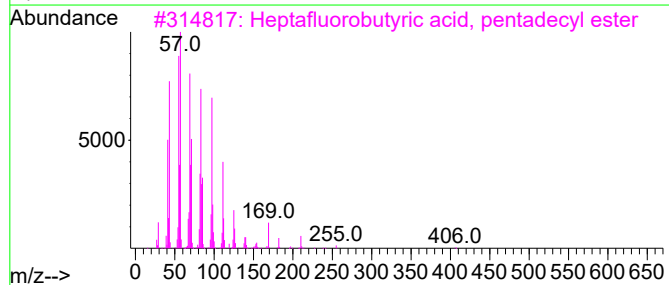
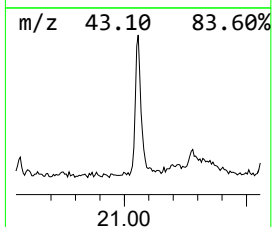
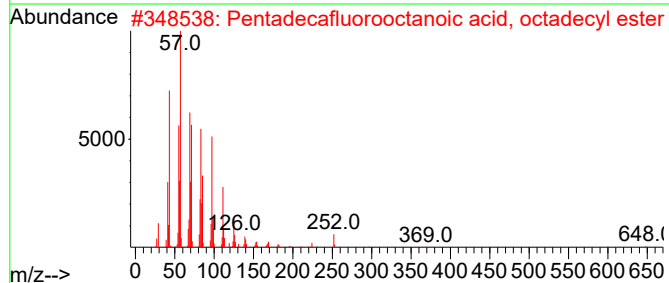
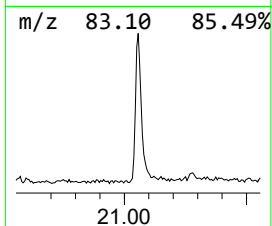
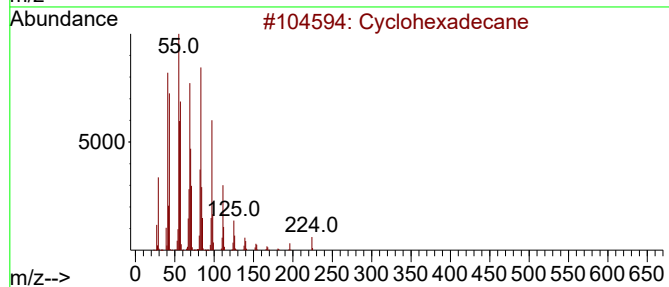
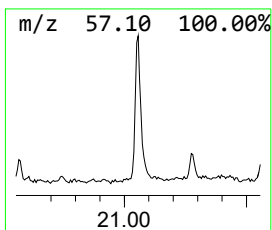
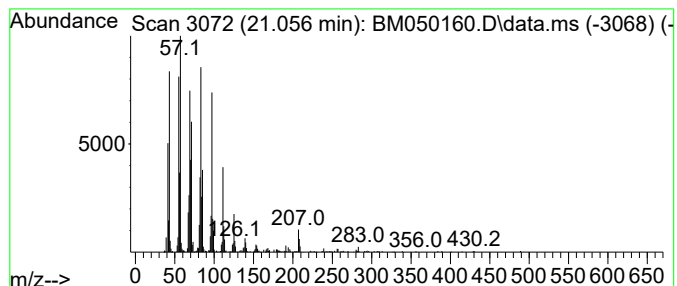
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclohexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.056	3.84 ng	619013	Chrysene-d12	21.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	95
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5			1-Heptacosanol	396	C27H56O	002004-39-9	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM050925\
Data File : BM050160.D
Acq On : 09 May 2025 15:27
Operator : RC/JU
Sample : Q1986-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-11

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	5.5	ng	532587	1	7.739	1955560	20.0
Benzophenone	15.751	5.9	ng	1120910	3	14.392	3828260	20.0
n-Hexadecanoic ...	18.039	12.7	ng	2756060	4	17.145	4332280	20.0
7-Hexadecene, (Z)-	18.904	2.1	ng	455666	4	17.145	4332280	20.0
Octadecanoic acid	19.321	5.5	ng	894575	5	21.386	3226350	20.0
1-Nonadecene	20.056	2.0	ng	325627	5	21.386	3226350	20.0
Cyclohexadecane	21.056	3.8	ng	619013	5	21.386	3226350	20.0