

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040225\
 Data File : BM049788.D
 Acq On : 02 Apr 2025 13:28
 Operator : RC/JU
 Sample : Q1679-05
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TP-9

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: BM049788.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	11	rVB	106083	128104	1.07%	0.185%
2	4.905	320	326	334	rVB	488304	662576	5.55%	0.955%
3	5.369	398	405	412	rBV	4493356	6122288	51.29%	8.822%
4	6.957	666	675	690	rBV	4304492	6432889	53.89%	9.269%
5	7.787	809	816	822	rBV	1047434	1568167	13.14%	2.260%
6	8.940	1005	1012	1020	rBV	2440497	3779406	31.66%	5.446%
7	10.581	1283	1291	1300	rBV	1211387	1970106	16.50%	2.839%
8	13.051	1703	1711	1718	rBV	6013786	8213882	68.81%	11.836%
9	14.427	1936	1945	1953	rBV	1862642	2572748	21.55%	3.707%
10	15.786	2169	2176	2185	rBV	649727	846789	7.09%	1.220%
11	15.916	2191	2198	2210	rBV	5383156	7053460	59.09%	10.164%
12	17.168	2405	2411	2416	rBV	2268378	3011702	25.23%	4.340%
13	18.074	2559	2565	2573	rBV	923678	1339049	11.22%	1.929%
14	18.139	2573	2576	2586	rVB	85096	172756	1.45%	0.249%
15	19.227	2756	2761	2769	rBV	166287	248696	2.08%	0.358%
16	19.351	2778	2782	2793	rBV	433793	696470	5.83%	1.004%
17	19.557	2812	2817	2820	rBV	241480	382427	3.20%	0.551%
18	19.586	2820	2822	2825	rVB	136162	148733	1.25%	0.214%
19	19.792	2852	2857	2864	rBV	10463574	11937389	100.00%	17.201%
20	20.486	2972	2975	2987	rVB	484756	605775	5.07%	0.873%
21	21.092	3074	3078	3087	rBV	478618	762219	6.39%	1.098%
22	21.315	3113	3116	3123	rVB	190199	222615	1.86%	0.321%
23	21.403	3124	3131	3135	rVV	2952977	4504543	37.73%	6.491%
24	21.445	3135	3138	3146	rVB	355713	546744	4.58%	0.788%
25	21.609	3163	3166	3178	rVB2	202665	295984	2.48%	0.426%
26	22.186	3259	3264	3266	rBV4	212957	395125	3.31%	0.569%
27	22.827	3370	3373	3378	rVB2	134044	202763	1.70%	0.292%
28	23.450	3475	3479	3485	rBV	193329	351851	2.95%	0.507%
29	24.397	3633	3640	3660	rVB	1603383	4224282	35.39%	6.087%

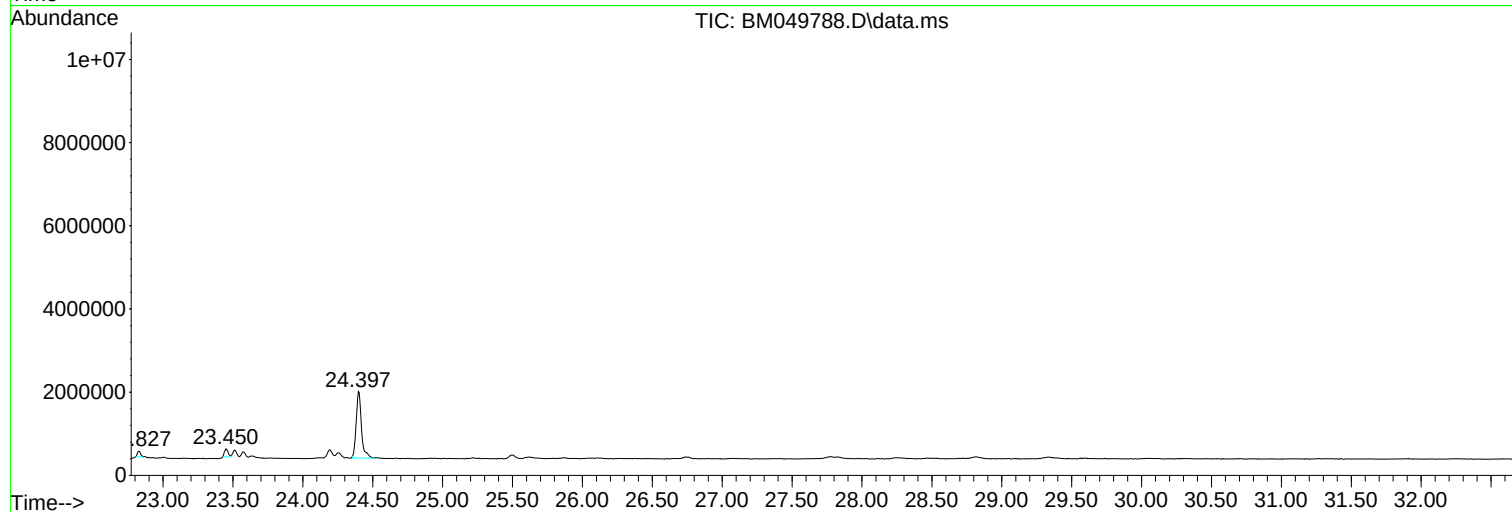
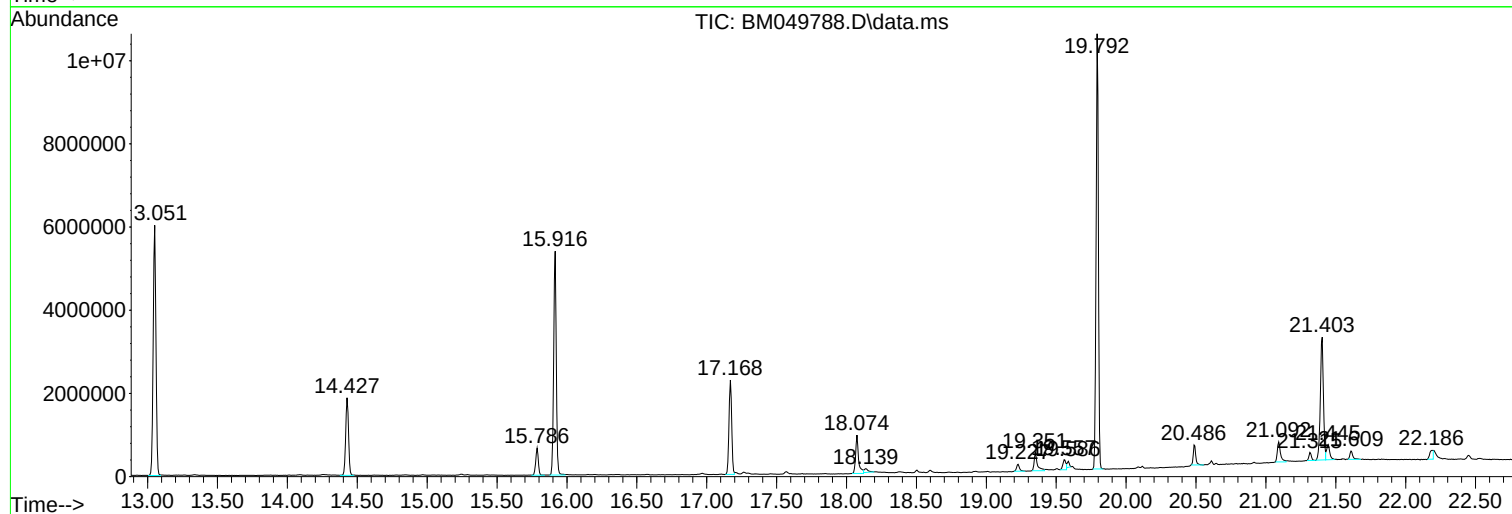
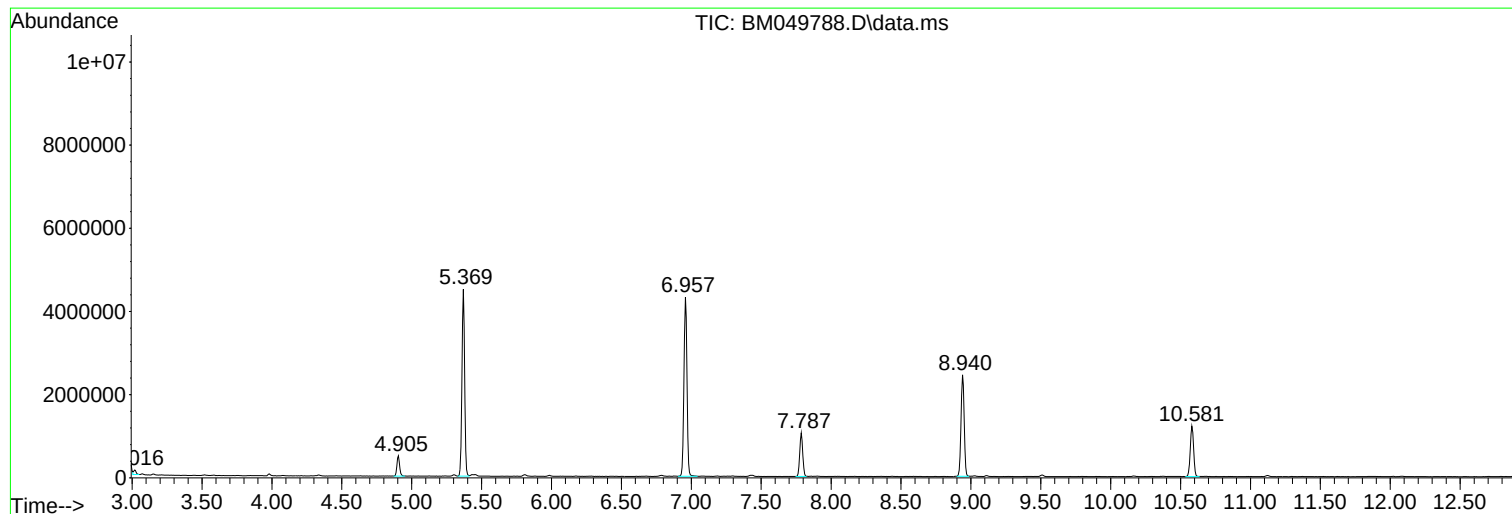
Sum of corrected areas: 69399538

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040225\
Data File : BM049788.D
Acq On : 02 Apr 2025 13:28
Operator : RC/JU
Sample : Q1679-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-9

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040225\
Data File : BM049788.D
Acq On : 02 Apr 2025 13:28
Operator : RC/JU
Sample : Q1679-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-9

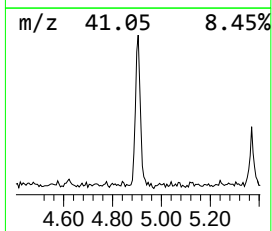
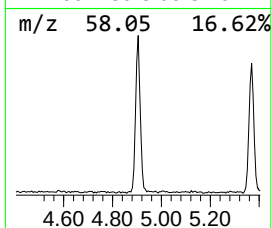
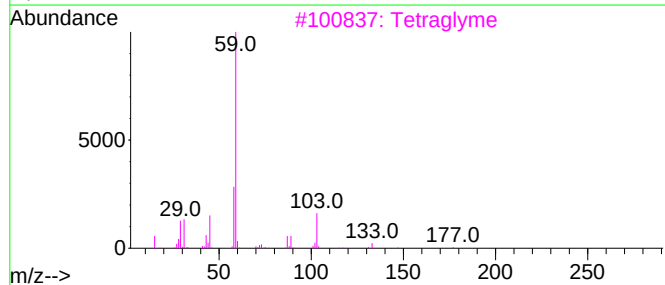
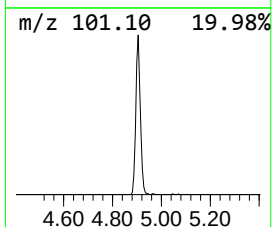
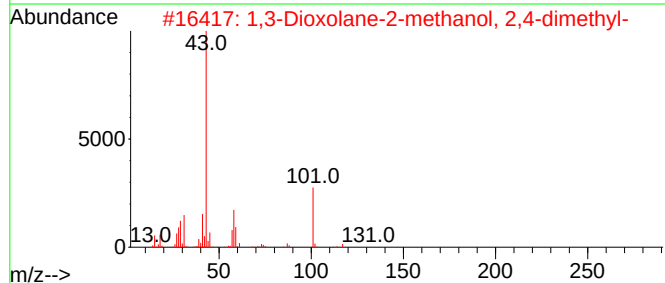
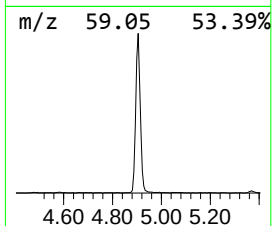
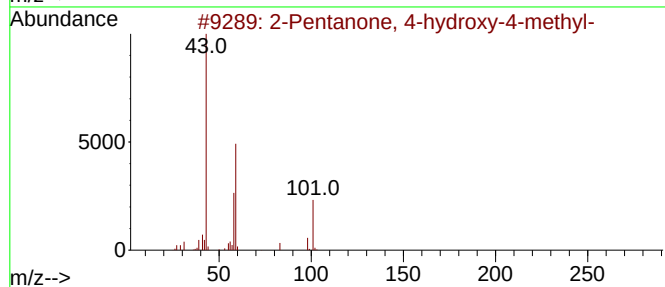
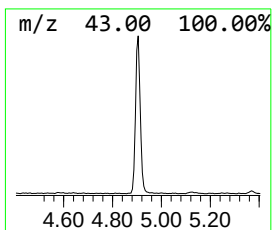
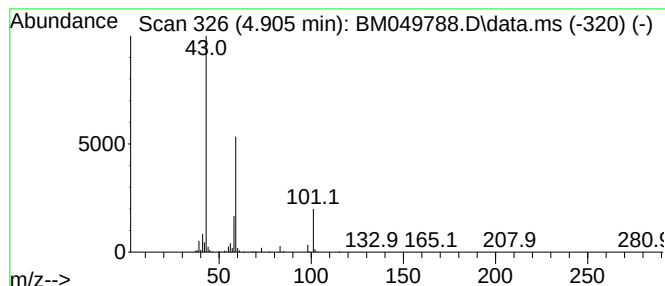
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.905	8.45 ng	662576	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	53		
2	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	28		
3	Tetraglyme	222	C10H22O5	000143-24-8	25		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040225\
Data File : BM049788.D
Acq On : 02 Apr 2025 13:28
Operator : RC/JU
Sample : Q1679-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-9

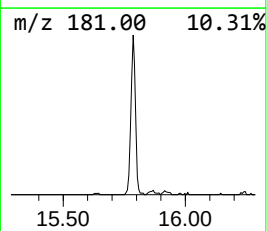
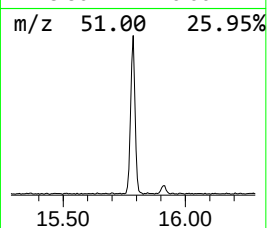
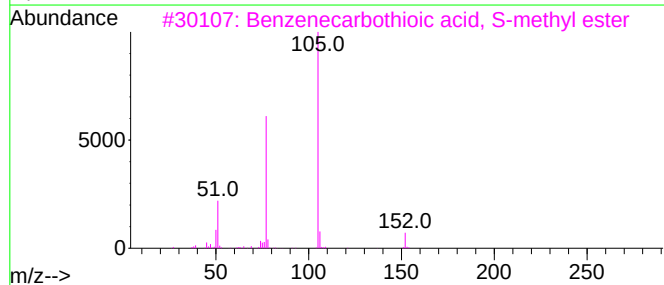
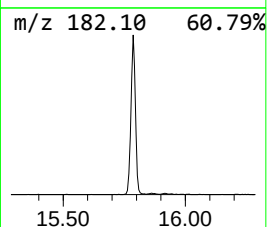
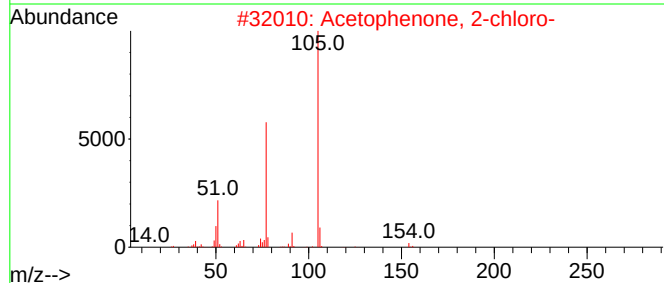
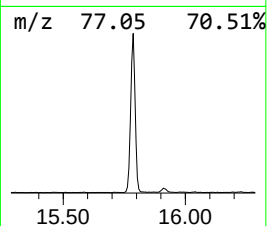
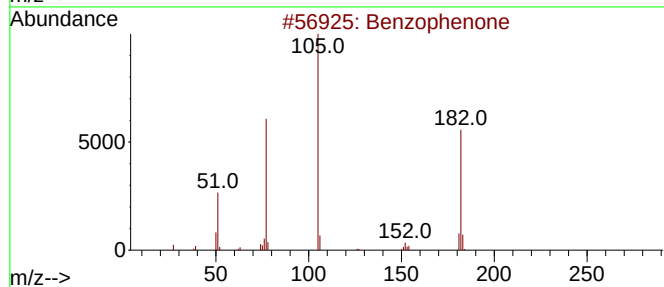
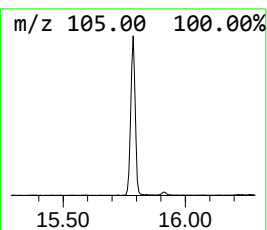
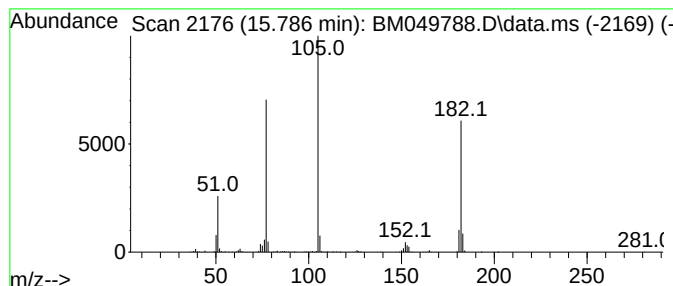
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.786	6.58 ng	846789	Acenaphthene-d10	14.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	49
5			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040225\
Data File : BM049788.D
Acq On : 02 Apr 2025 13:28
Operator : RC/JU
Sample : Q1679-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-9

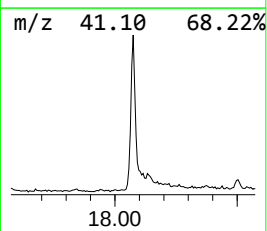
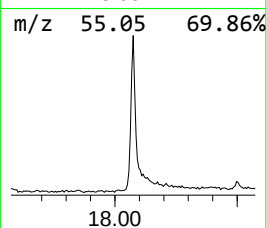
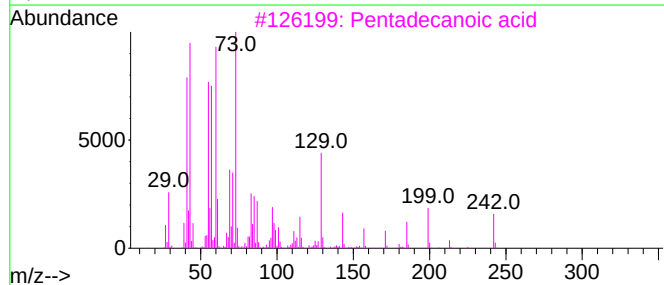
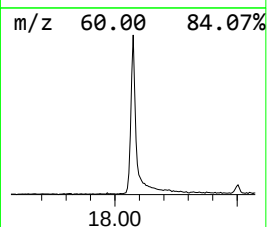
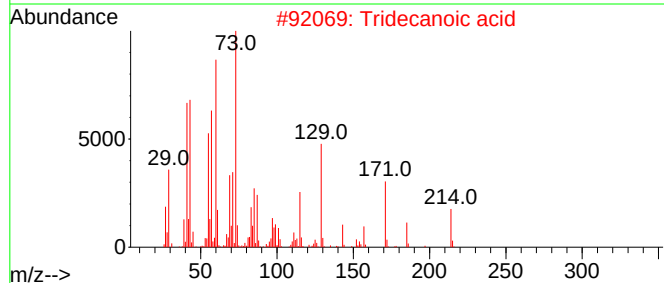
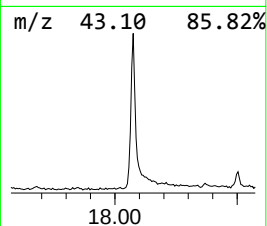
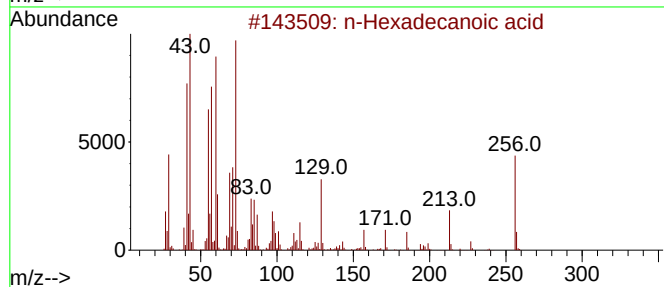
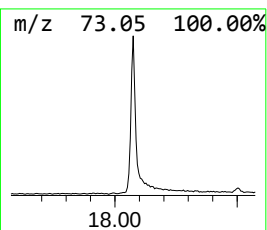
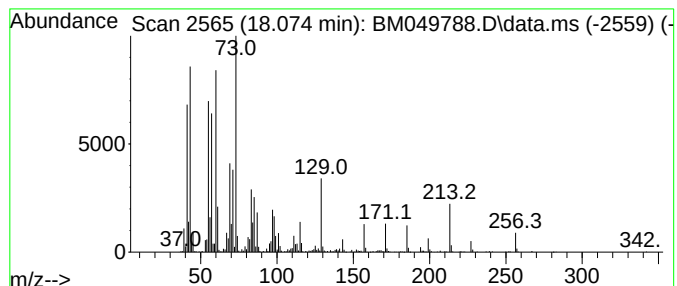
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.074	8.89 ng	1339050	Phenanthrene-d10	17.168

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040225\
Data File : BM049788.D
Acq On : 02 Apr 2025 13:28
Operator : RC/JU
Sample : Q1679-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-9

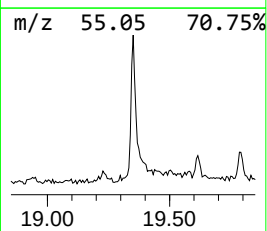
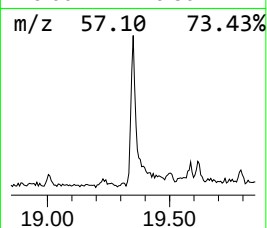
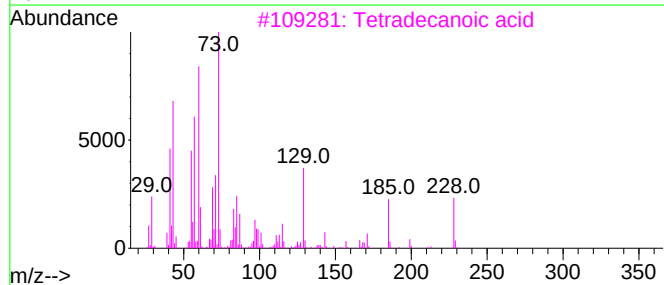
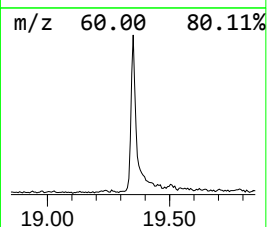
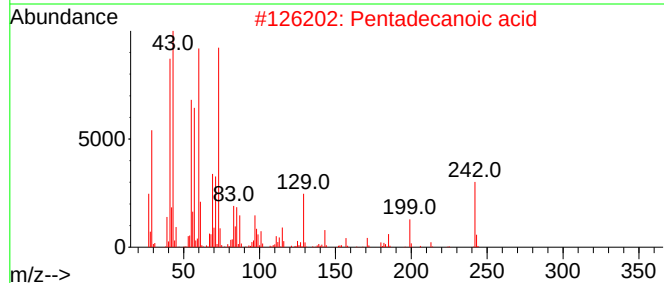
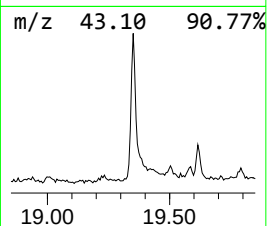
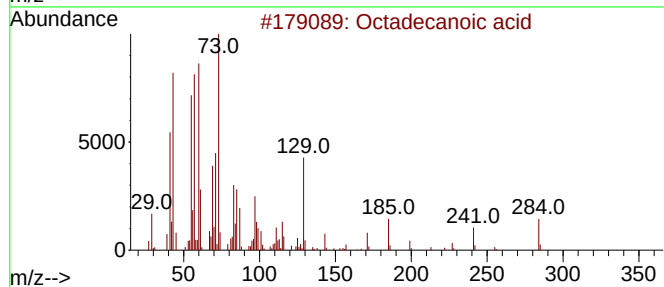
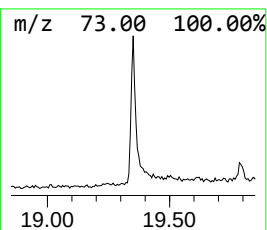
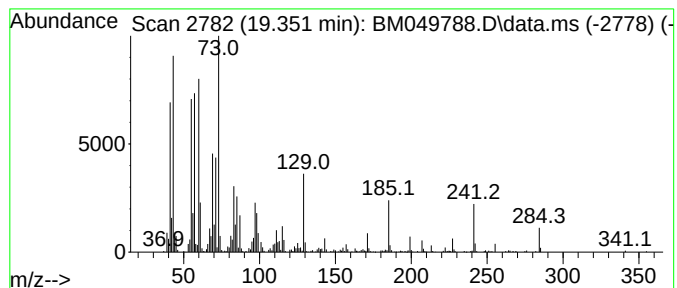
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.351	3.09 ng	696470	Chrysene-d12	21.403

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	81
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	49
5			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040225\
Data File : BM049788.D
Acq On : 02 Apr 2025 13:28
Operator : RC/JU
Sample : Q1679-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-9

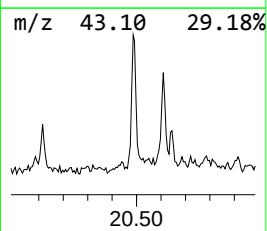
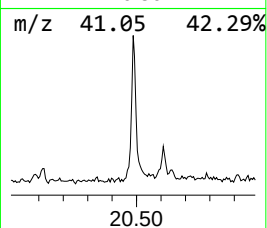
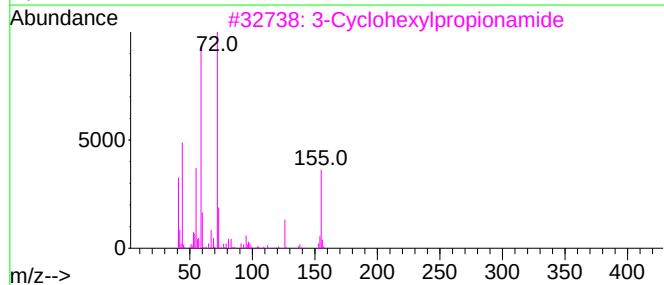
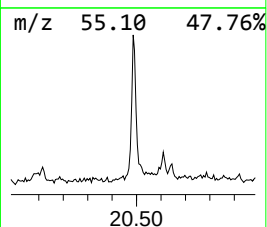
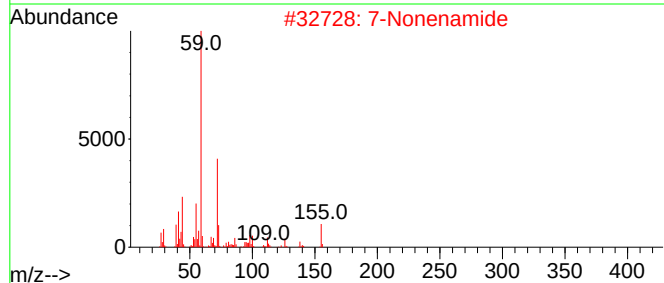
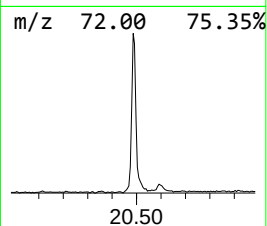
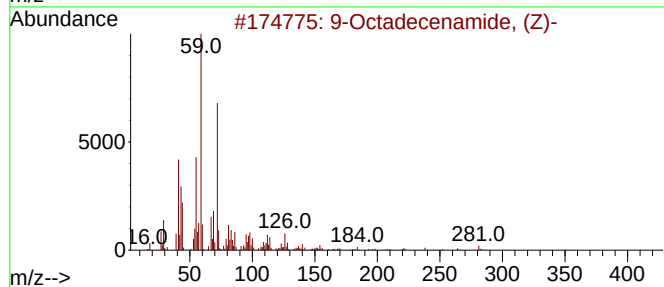
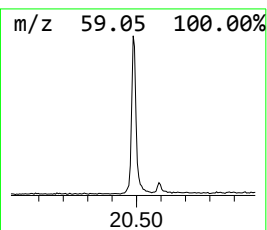
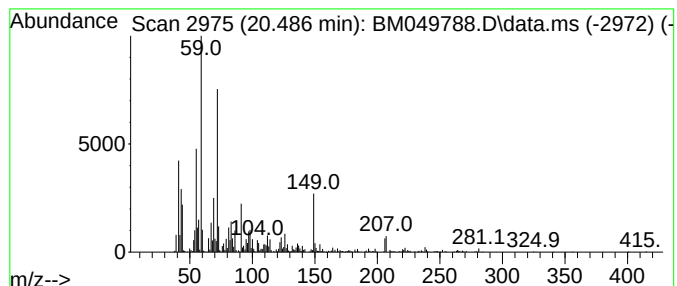
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.486	2.69 ng	605775	Chrysene-d12	21.403

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2			7-Nonenamide	155	C9H17NO	090949-53-4	64
3			3-Cyclohexylpropionamide	155	C9H17NO	004361-29-9	47
4			Palmitoleamide	253	C16H31NO	106010-22-4	35
5			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040225\
Data File : BM049788.D
Acq On : 02 Apr 2025 13:28
Operator : RC/JU
Sample : Q1679-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-9

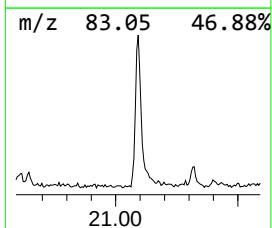
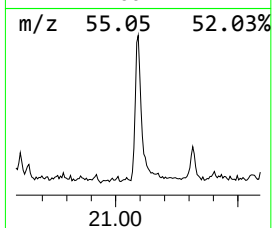
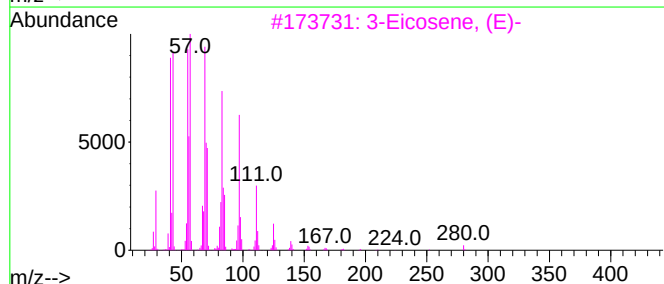
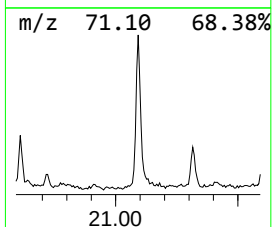
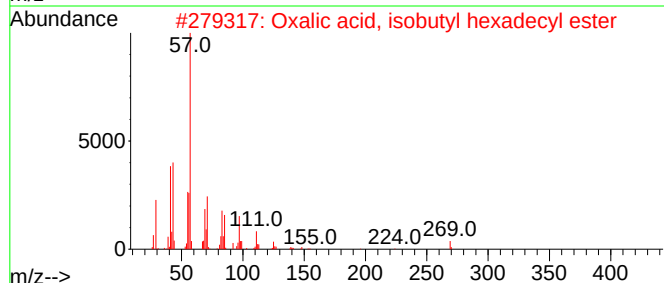
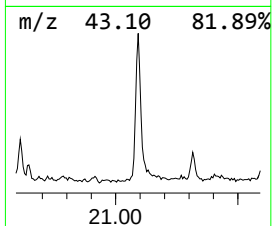
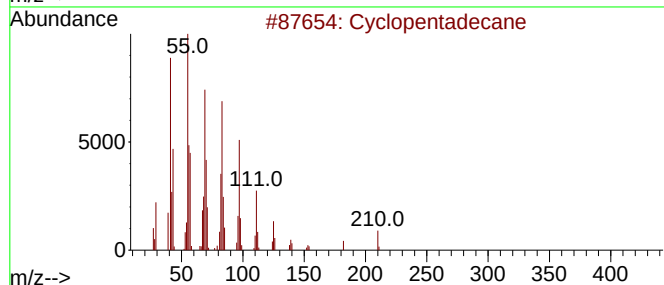
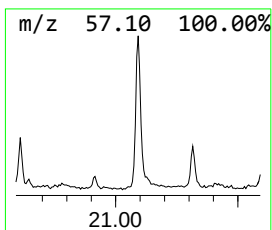
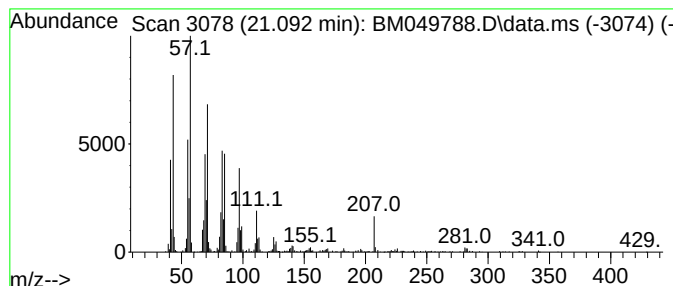
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclopentadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.092	3.38 ng	762219	Chrysene-d12	21.403

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	92
2			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
3			3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4			Oxalic acid, hexadecyl propyl ester	356	C21H40O4	1000309-26-9	90
5			Hexadecane	226	C16H34	000544-76-3	84



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040225\
Data File : BM049788.D
Acq On : 02 Apr 2025 13:28
Operator : RC/JU
Sample : Q1679-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-9

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
2-Pentanone, 4-...	4.905	8.4	ng	662576	1	7.787	1568170	20.0
Benzophenone	15.786	6.6	ng	846789	3	14.427	2572750	20.0
n-Hexadecanoic ...	18.074	8.9	ng	1339050	4	17.168	3011700	20.0
Octadecanoic acid	19.351	3.1	ng	696470	5	21.403	4504540	20.0
9-Octadecenamid...	20.486	2.7	ng	605775	5	21.403	4504540	20.0
Cyclopentadecane	21.092	3.4	ng	762219	5	21.403	4504540	20.0