

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041025\
 Data File : BM049883.D
 Acq On : 10 Apr 2025 14:10
 Operator : RC/JU
 Sample : Q1752-07
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TP-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-BM040825.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM049883.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	319	324	336	rVB	795234	1056470	9.86%	1.774%
2	5.357	397	403	420	rVB	3219946	4586031	42.79%	7.702%
3	5.969	502	507	516	rVB	118323	181130	1.69%	0.304%
4	6.951	666	674	691	rBV	3013002	4852482	45.28%	8.149%
5	7.775	807	814	823	rBV	933228	1440372	13.44%	2.419%
6	8.928	1002	1010	1022	rBV	1765468	2846703	26.56%	4.781%
7	10.569	1281	1289	1302	rBV	1079618	1826511	17.04%	3.067%
8	13.039	1702	1709	1725	rBV	5072003	7157401	66.78%	12.020%
9	14.416	1937	1943	1951	rBV	1677834	2508451	23.41%	4.213%
10	15.774	2167	2174	2181	rBV	937493	1245187	11.62%	2.091%
11	15.904	2189	2196	2219	rBV	4564256	6153753	57.42%	10.335%
12	16.339	2265	2270	2279	rVB	87885	130526	1.22%	0.219%
13	17.157	2402	2409	2414	rBV2	2096191	3027306	28.25%	5.084%
14	17.198	2414	2416	2423	rVV	344965	455893	4.25%	0.766%
15	17.286	2423	2431	2436	rVB3	73767	144432	1.35%	0.243%
16	18.057	2554	2562	2572	rBV2	352727	703232	6.56%	1.181%
17	19.215	2754	2759	2766	rBV	839745	1075941	10.04%	1.807%
18	19.339	2776	2780	2787	rBV2	109818	161493	1.51%	0.271%
19	19.580	2812	2821	2829	rBV	737179	1129769	10.54%	1.897%
20	19.786	2850	2856	2867	rVB	9187614	10717225	100.00%	17.998%
21	21.080	3072	3076	3083	rBV3	235912	390988	3.65%	0.657%
22	21.392	3122	3129	3134	rBV2	2426098	3936959	36.73%	6.612%
23	21.439	3134	3137	3147	rVB	316708	481845	4.50%	0.809%
24	24.392	3631	3639	3647	rBV	1342862	3335303	31.12%	5.601%

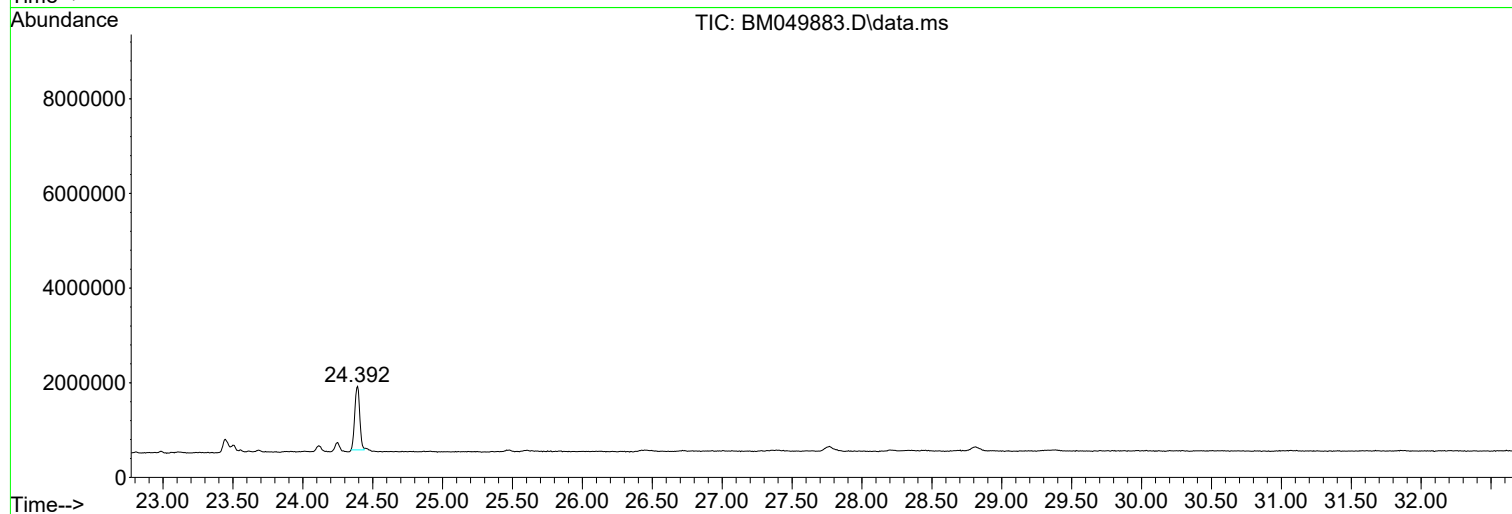
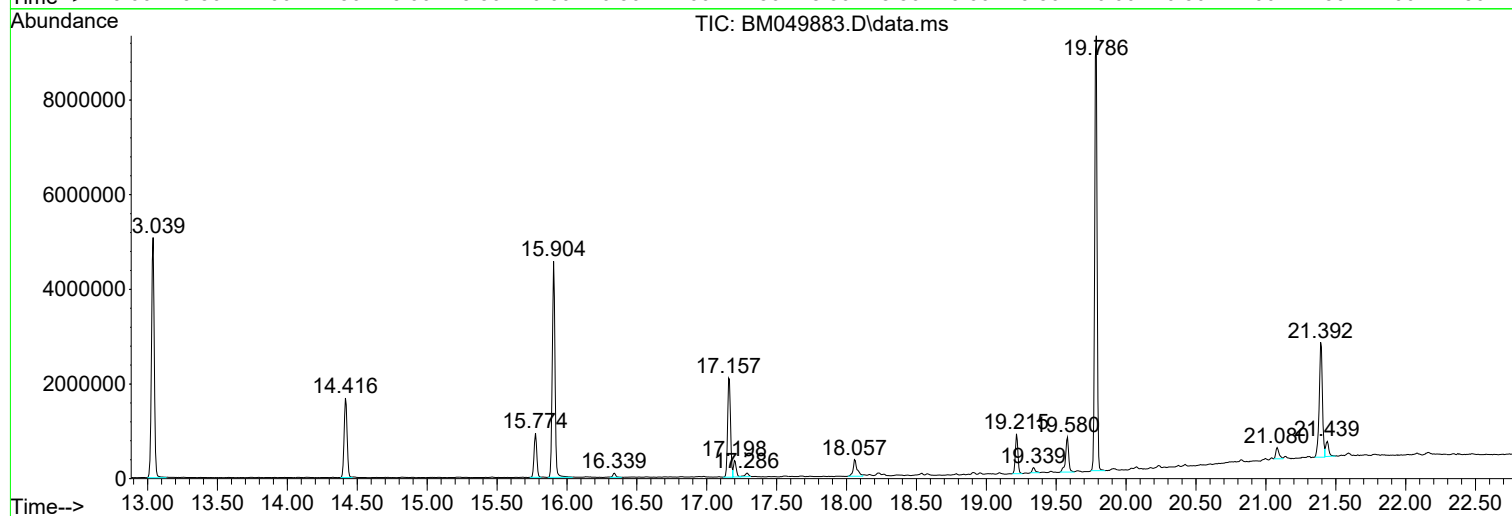
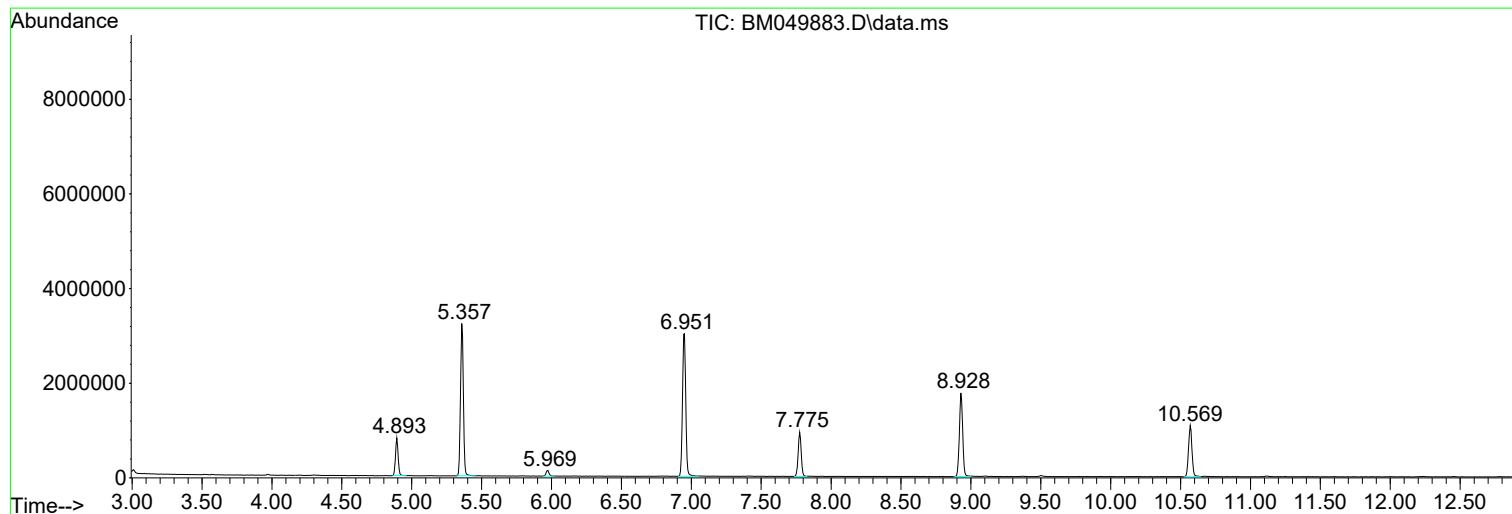
Sum of corrected areas: 59545403

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041025\
Data File : BM049883.D
Acq On : 10 Apr 2025 14:10
Operator : RC/JU
Sample : Q1752-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-3

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041025\
Data File : BM049883.D
Acq On : 10 Apr 2025 14:10
Operator : RC/JU
Sample : Q1752-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-3

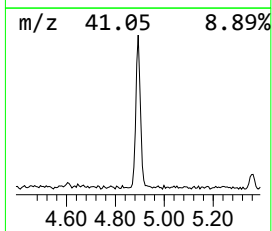
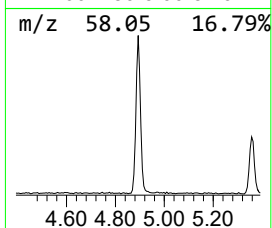
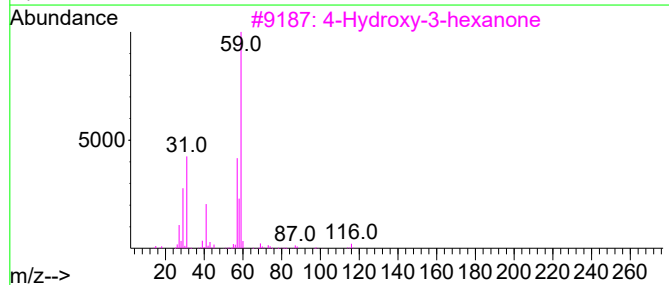
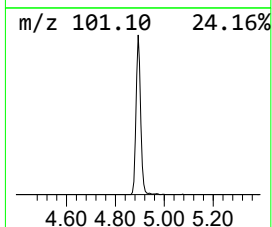
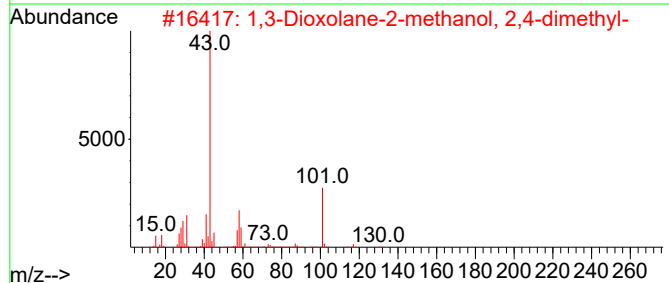
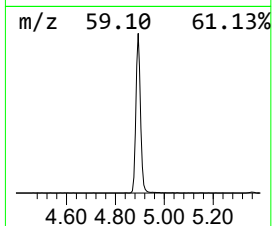
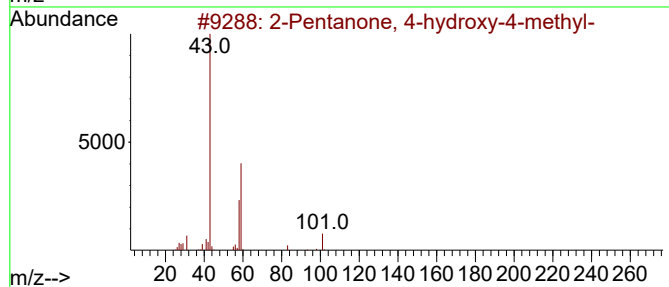
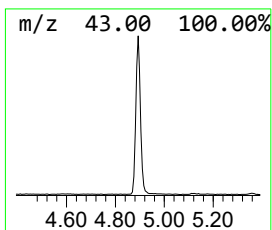
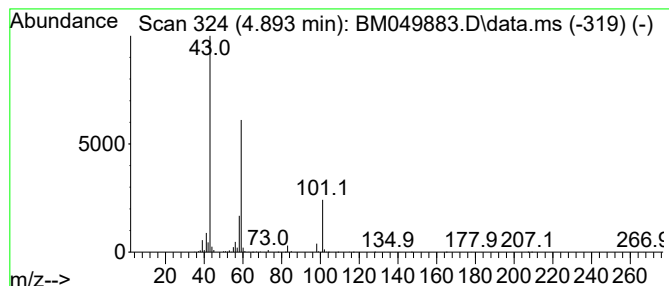
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.893	14.67 ng	1056470	1,4-Dichlorobenzene-d4	7.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25		
3	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	17		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041025\
Data File : BM049883.D
Acq On : 10 Apr 2025 14:10
Operator : RC/JU
Sample : Q1752-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-3

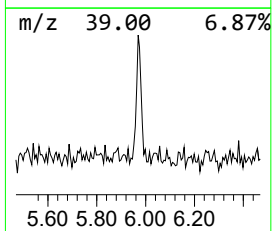
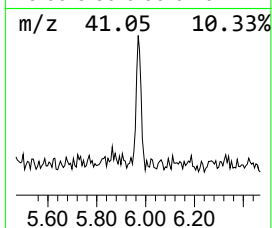
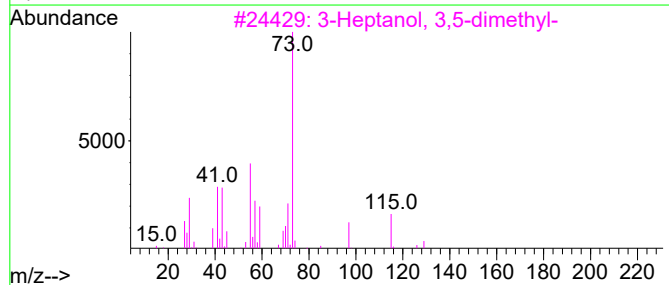
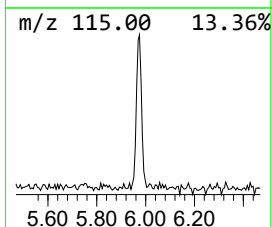
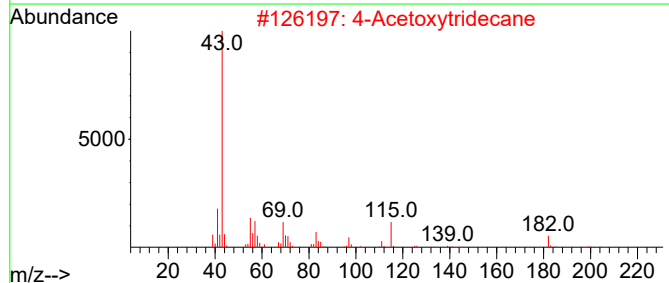
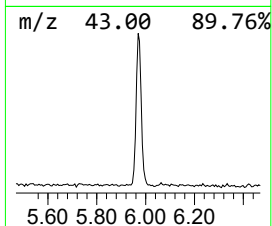
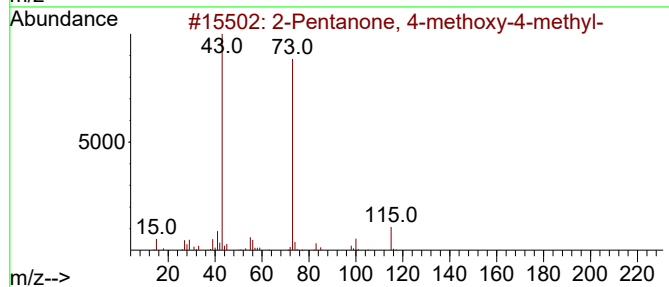
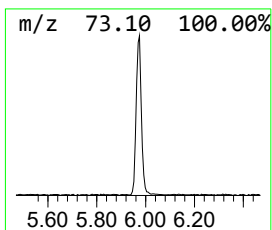
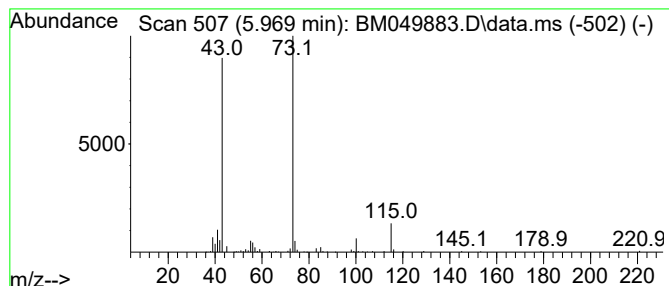
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.969	2.52 ng	181130	1,4-Dichlorobenzene-d4	7.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2			4-Acetoxytridecane	242	C15H30O2	060826-30-4	25
3			3-Heptanol, 3,5-dimethyl-	144	C9H20O	019549-74-7	25
4			3-Hexanol, acetate	144	C8H16O2	040780-64-1	25
5			2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041025\
Data File : BM049883.D
Acq On : 10 Apr 2025 14:10
Operator : RC/JU
Sample : Q1752-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-3

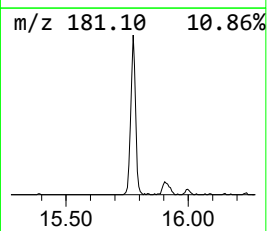
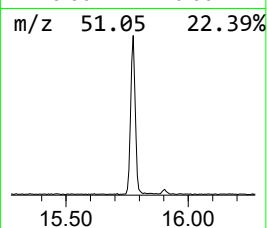
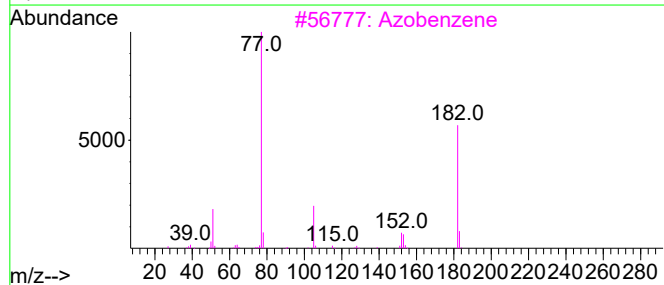
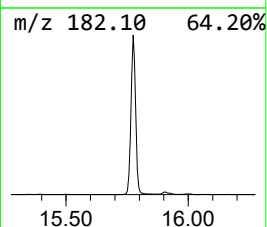
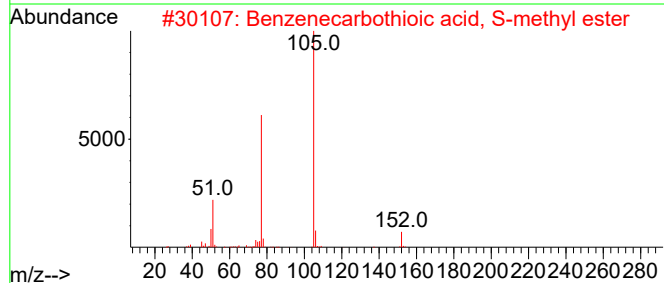
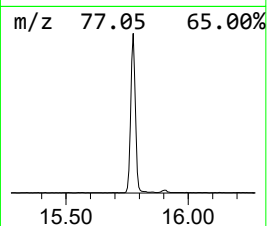
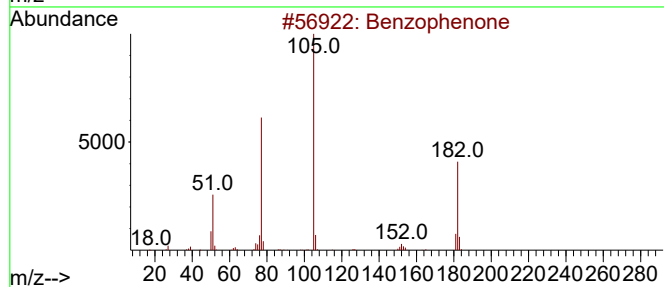
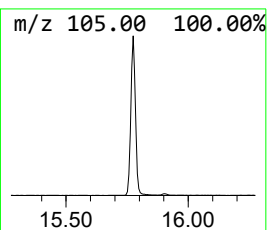
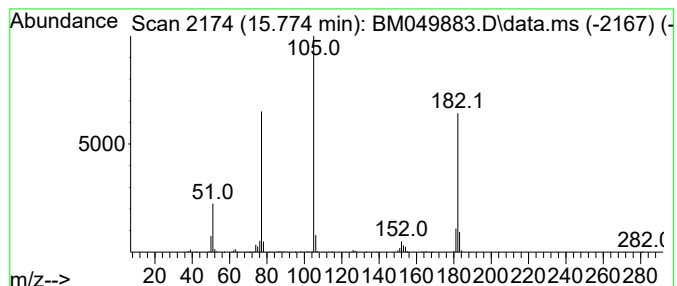
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.774	9.93 ng	1245190	Acenaphthene-d10	14.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
3			Azobenzene	182	C12H10N2	000103-33-3	47
4			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
5			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041025\
Data File : BM049883.D
Acq On : 10 Apr 2025 14:10
Operator : RC/JU
Sample : Q1752-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-3

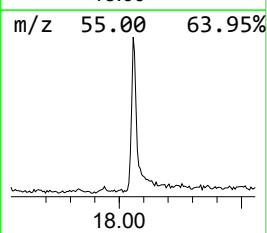
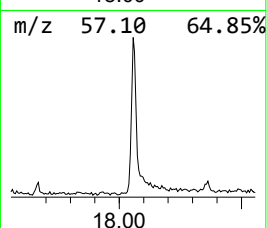
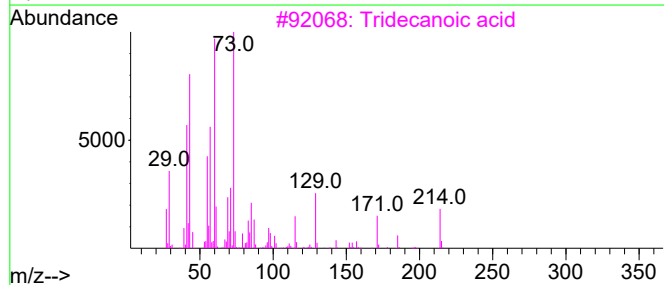
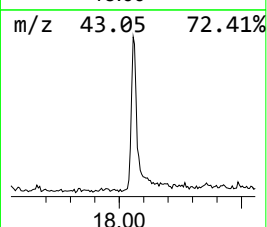
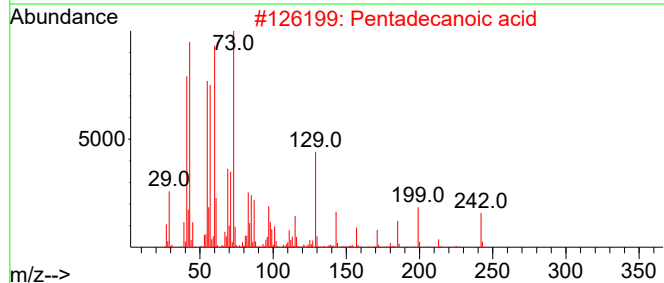
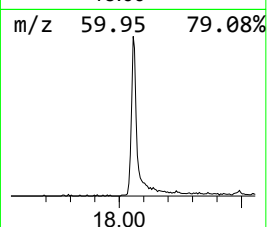
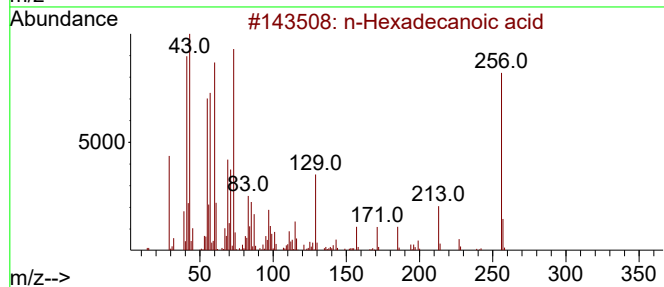
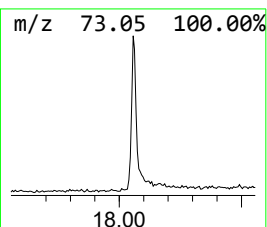
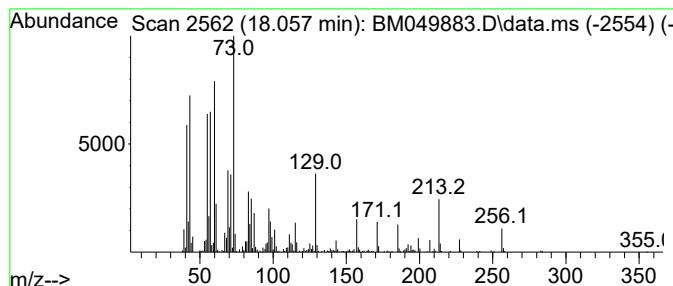
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.057	4.65 ng	703232	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	89
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5		Octadecanoic acid	284	C18H36O2	000057-11-4	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041025\
Data File : BM049883.D
Acq On : 10 Apr 2025 14:10
Operator : RC/JU
Sample : Q1752-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-3

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.893	14.7	ng	1056470	1	7.775	1440370	20.0
2-Pentanone, 4-...	5.969	2.5	ng	181130	1	7.775	1440370	20.0
Benzophenone	15.774	9.9	ng	1245190	3	14.416	2508450	20.0
n-Hexadecanoic ...	18.057	4.7	ng	703232	4	17.157	3027310	20.0