

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
 Data File : BM047407.D
 Acq On : 30 Aug 2024 15:40
 Operator : RC/JU
 Sample : P3799-03
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TEST-PITS-4

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-BM082624.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047407.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.557	277	284	293	rBV	208645	296974	4.44%	0.683%
2	5.004	354	360	379	rBV	2189375	3430622	51.27%	7.892%
3	6.569	619	626	641	rBV	2069279	3537192	52.87%	8.137%
4	7.345	751	758	768	rBV	720033	1162761	17.38%	2.675%
5	8.492	946	953	973	rBV	1408382	2444631	36.54%	5.624%
6	9.081	1045	1053	1062	rBV	48021	113802	1.70%	0.262%
7	10.098	1219	1226	1243	rBV	882855	1544341	23.08%	3.553%
8	12.610	1646	1653	1675	rBV	3496778	5411276	80.88%	12.449%
9	13.927	1870	1877	1884	rBV3	25931	76092	1.14%	0.175%
10	14.004	1884	1890	1908	rVB	1292496	2133192	31.88%	4.907%
11	15.392	2120	2126	2142	rBV	1357876	2059373	30.78%	4.738%
12	15.521	2142	2148	2169	rVV	2615639	4112007	61.46%	9.460%
13	15.957	2217	2222	2229	rBV	241265	335017	5.01%	0.771%
14	16.774	2355	2361	2374	rVB	1638963	2417122	36.13%	5.561%
15	17.709	2515	2520	2543	rVB	683513	1362515	20.36%	3.134%
16	17.974	2560	2565	2577	rBV3	41824	105710	1.58%	0.243%
17	18.392	2632	2636	2643	rBV9	33361	72455	1.08%	0.167%
18	18.539	2656	2661	2666	rVB2	65126	115423	1.73%	0.266%
19	18.856	2711	2715	2719	rBV	93358	151891	2.27%	0.349%
20	18.933	2725	2728	2736	rVB3	76094	137436	2.05%	0.316%
21	19.009	2737	2741	2757	rVV2	267949	459901	6.87%	1.058%
22	19.227	2774	2778	2783	rVB	114800	161459	2.41%	0.371%
23	19.439	2809	2814	2826	rBV	5294361	6690673	100.00%	15.392%
24	19.903	2890	2893	2900	rVB8	61219	83715	1.25%	0.193%
25	20.744	3032	3036	3043	rBV	429149	613761	9.17%	1.412%
26	21.021	3078	3083	3088	rBV	1665065	2251847	33.66%	5.180%
27	23.721	3535	3542	3554	rVB	927111	2187501	32.69%	5.032%

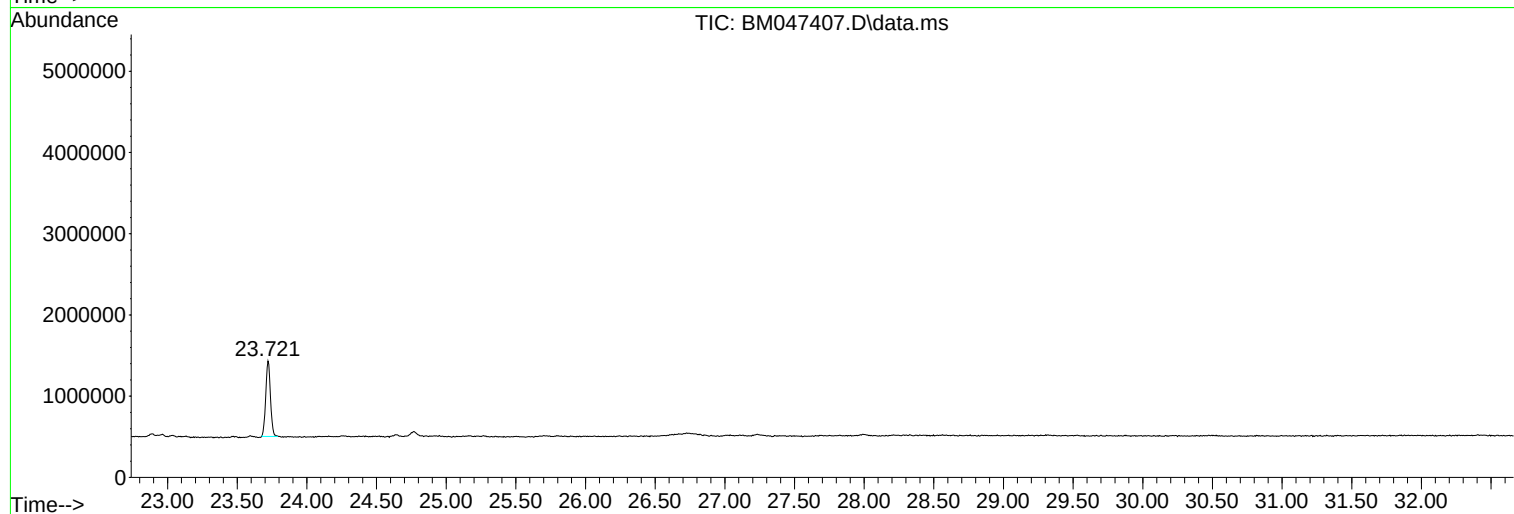
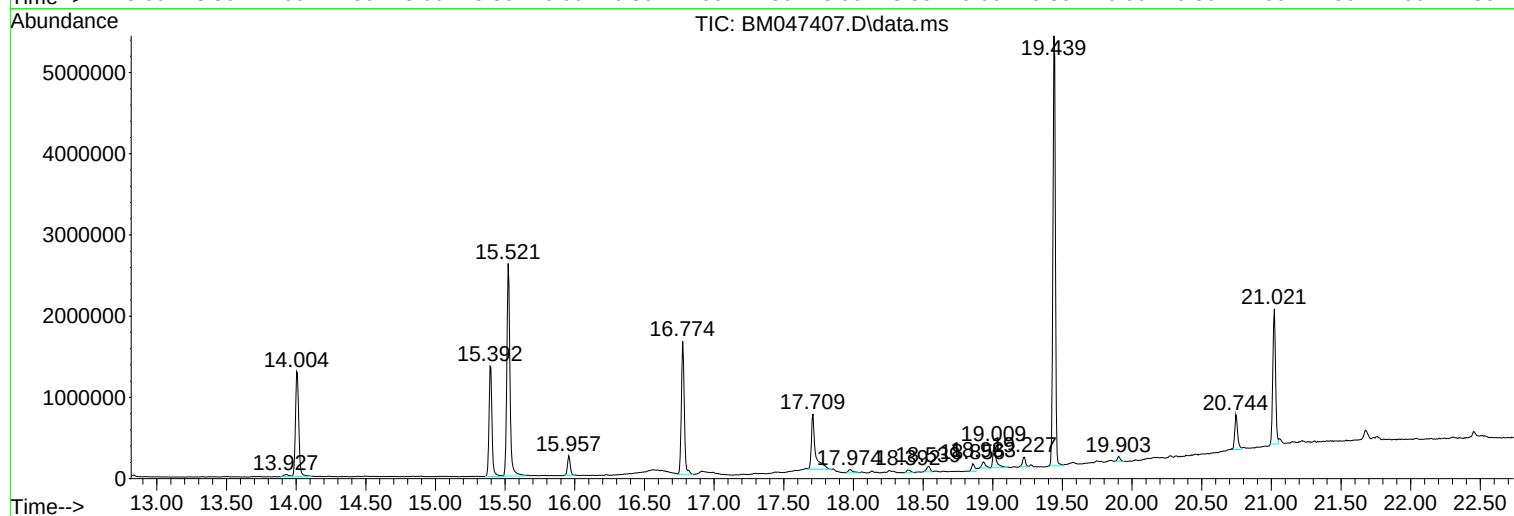
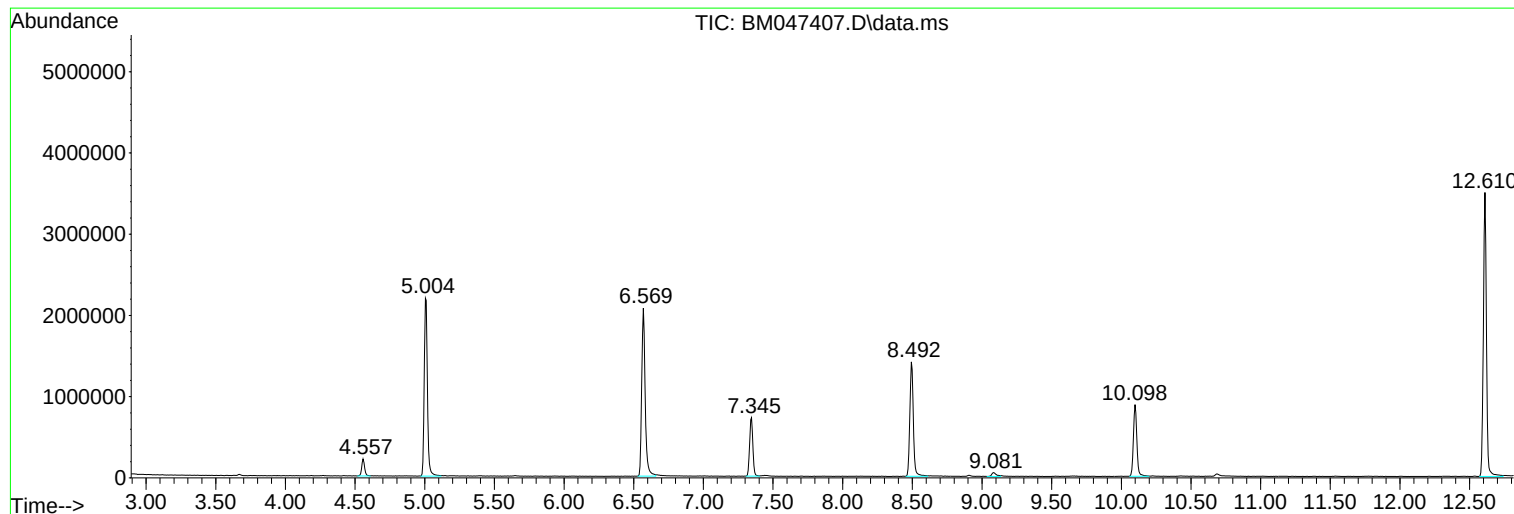
Sum of corrected areas: 43468689

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047407.D
Acq On : 30 Aug 2024 15:40
Operator : RC/JU
Sample : P3799-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TEST-PITS-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.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\BM083024\
Data File : BM047407.D
Acq On : 30 Aug 2024 15:40
Operator : RC/JU
Sample : P3799-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TEST-PITS-4

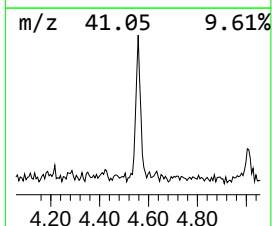
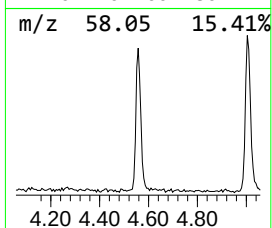
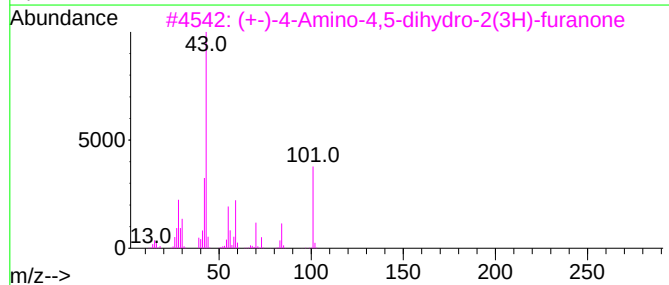
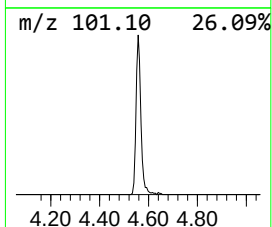
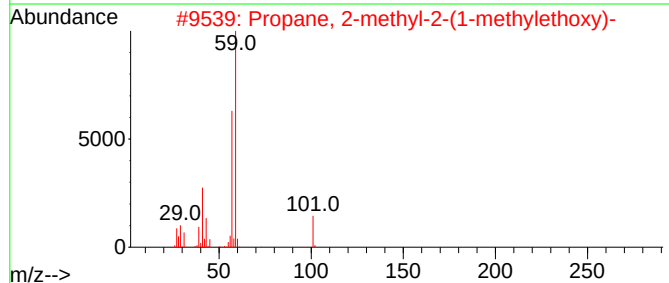
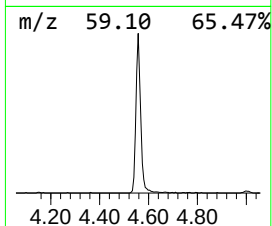
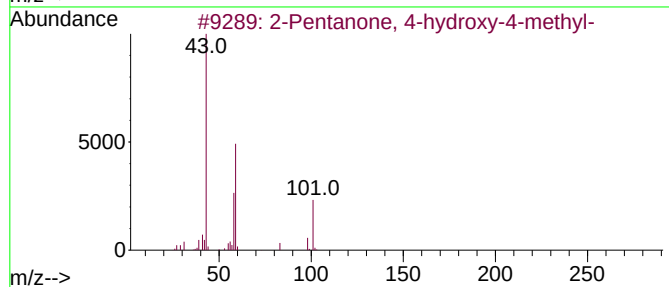
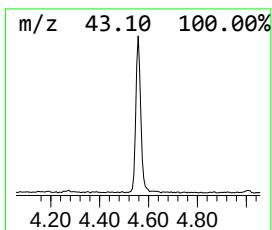
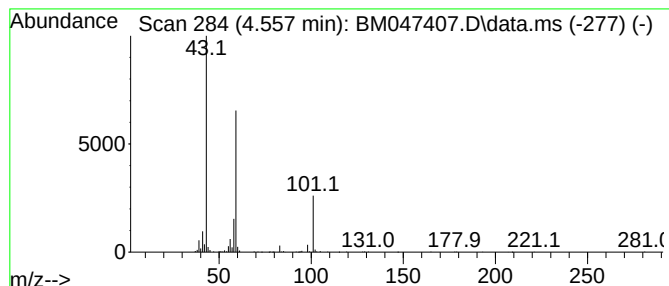
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.557	5.11 ng	296974	1,4-Dichlorobenzene-d4	7.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42		
3	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	25		
4	Tetraglyme	222	C10H22O5	000143-24-8	25		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047407.D
Acq On : 30 Aug 2024 15:40
Operator : RC/JU
Sample : P3799-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TEST-PITS-4

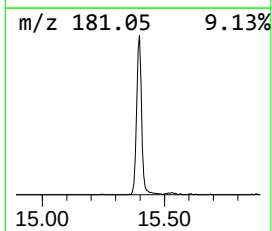
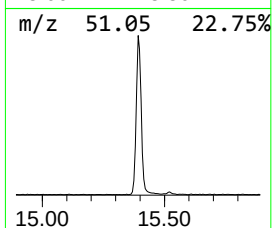
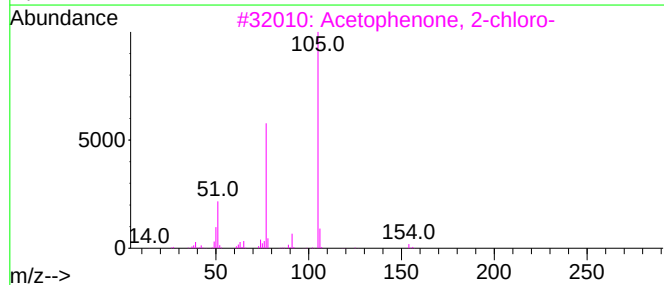
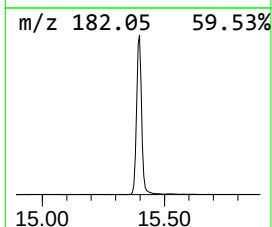
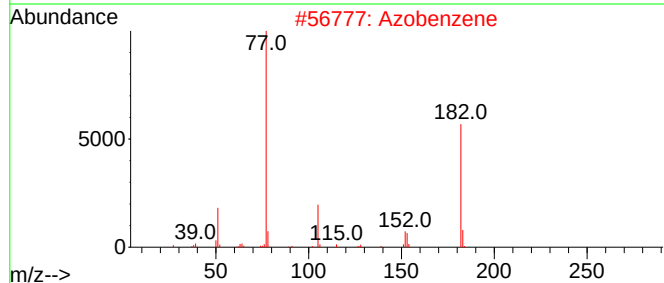
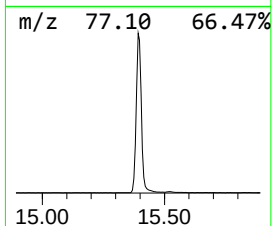
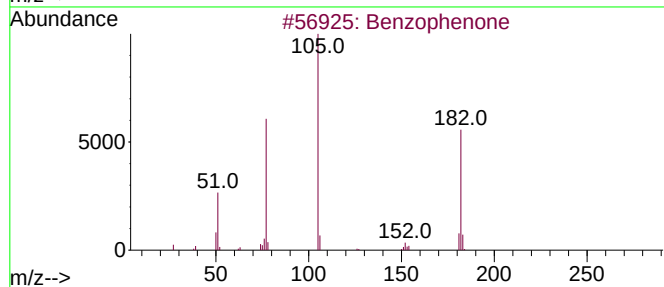
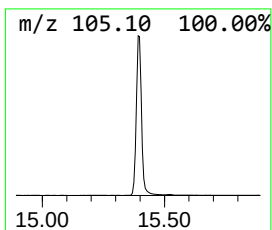
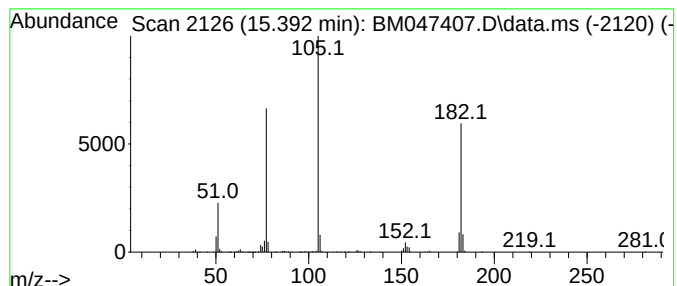
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.392	17.04 ng	2059370	Phenanthrene-d10	16.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	64
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	49
5			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047407.D
Acq On : 30 Aug 2024 15:40
Operator : RC/JU
Sample : P3799-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TEST-PITS-4

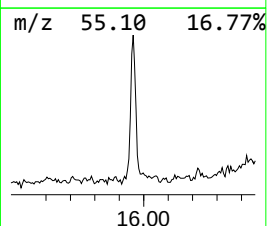
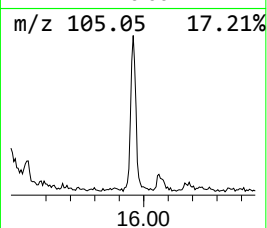
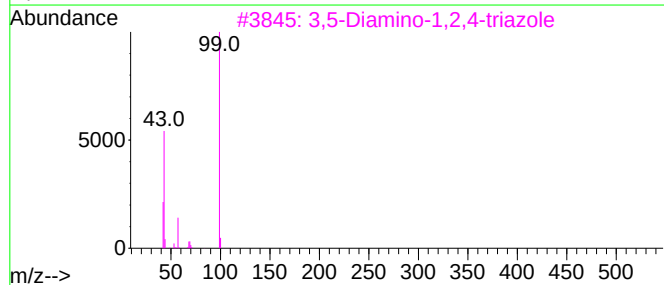
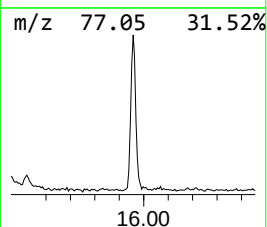
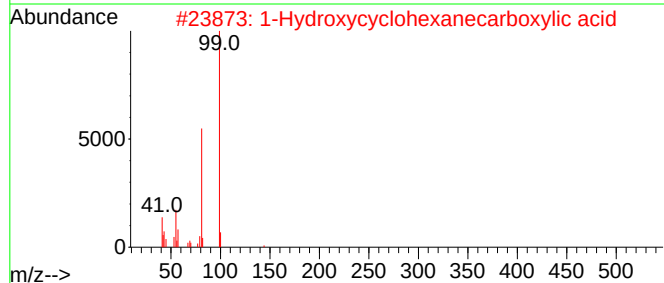
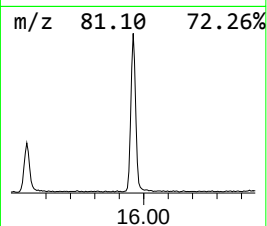
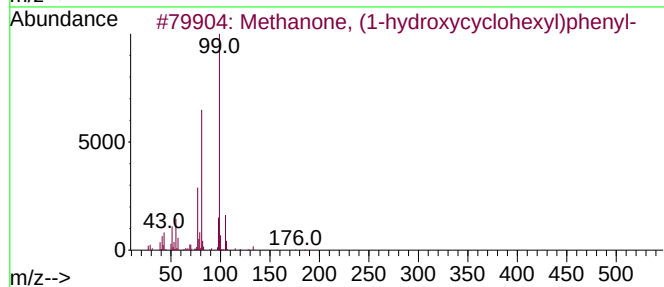
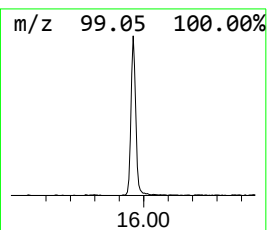
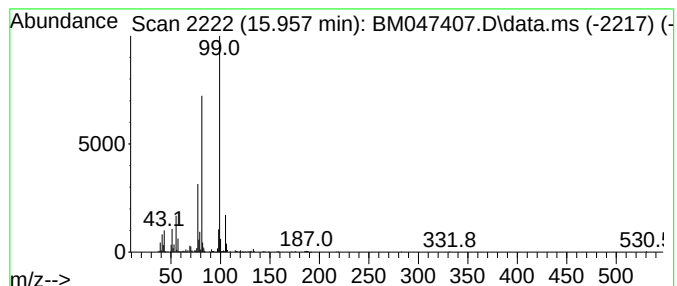
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Methanone, (1-hydroxycyclohexyl) Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.957	2.77 ng	335017	Phenanthrene-d10	16.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	90
2			1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	50
3			3,5-Diamino-1,2,4-triazole	99	C2H5N5	001455-77-2	43
4			Hexanoic acid, thio-, S-butyl ester	188	C10H20O5	002432-79-3	38
5			1,1'-Bicyclohexyl-1,1'-diol	198	C12H22O2	002888-11-1	33



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047407.D
Acq On : 30 Aug 2024 15:40
Operator : RC/JU
Sample : P3799-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TEST-PITS-4

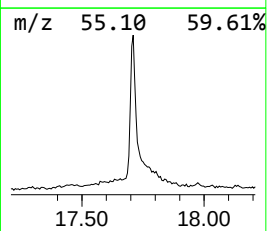
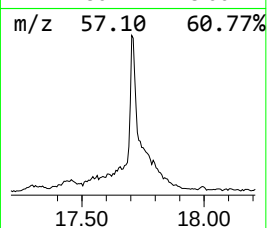
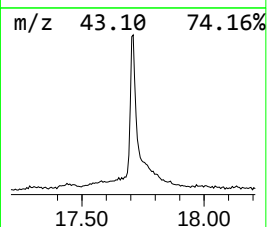
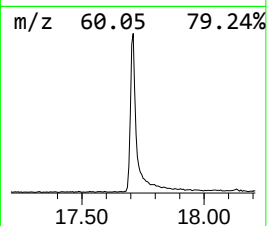
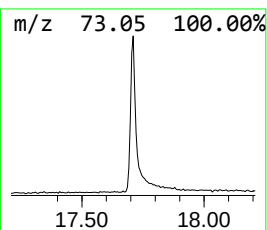
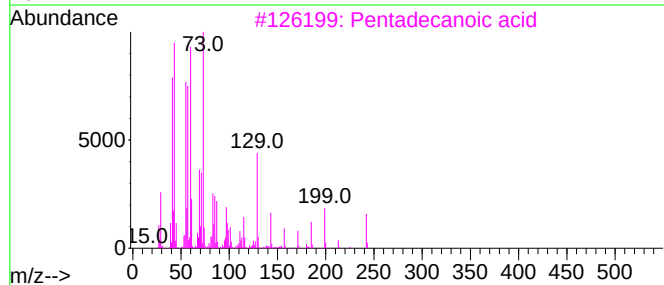
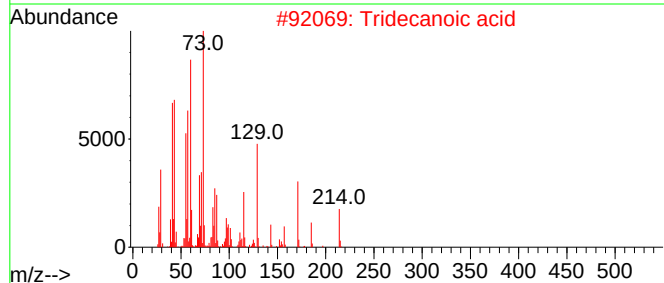
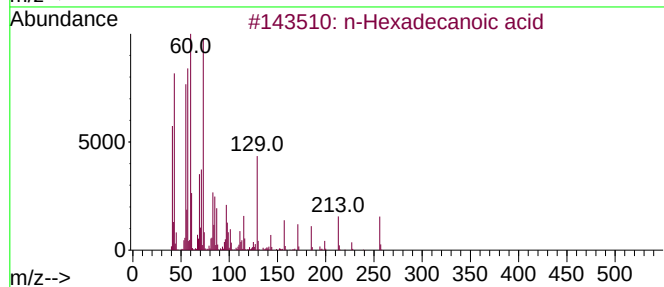
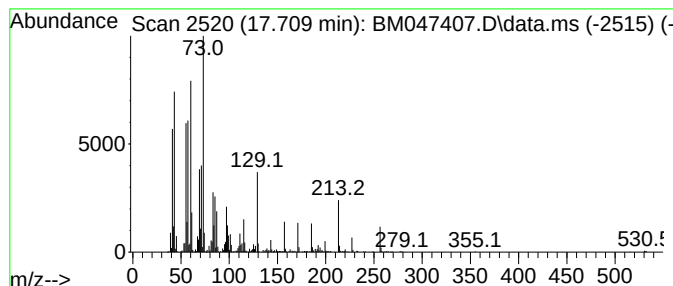
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.709	11.27 ng	1362520	Phenanthrene-d10	16.774

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	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Octadecanoic acid	284	C18H36O2	000057-11-4	81
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047407.D
Acq On : 30 Aug 2024 15:40
Operator : RC/JU
Sample : P3799-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TEST-PITS-4

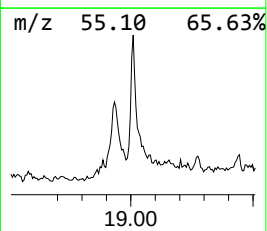
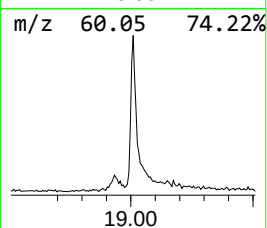
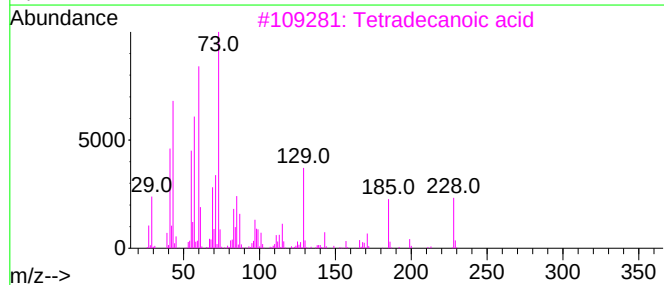
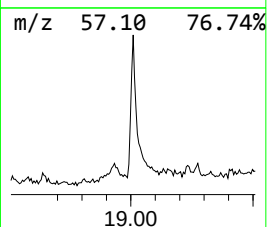
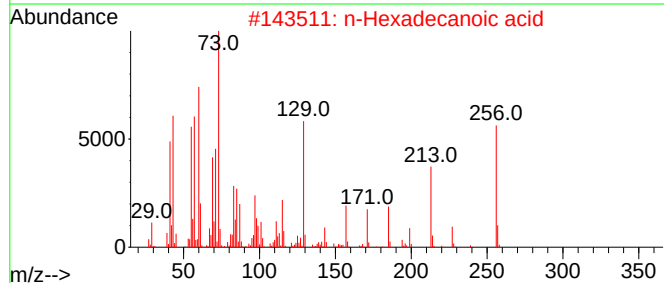
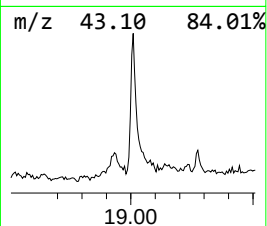
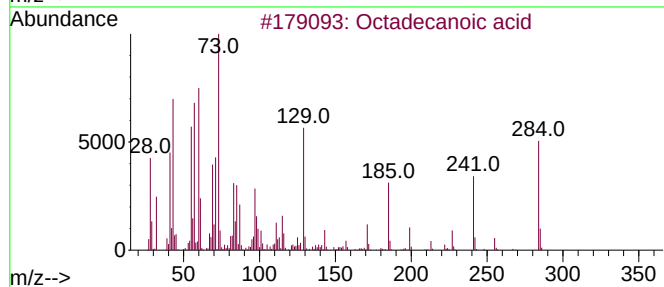
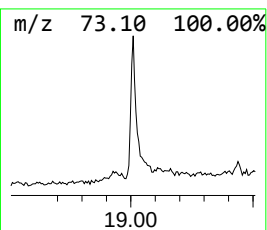
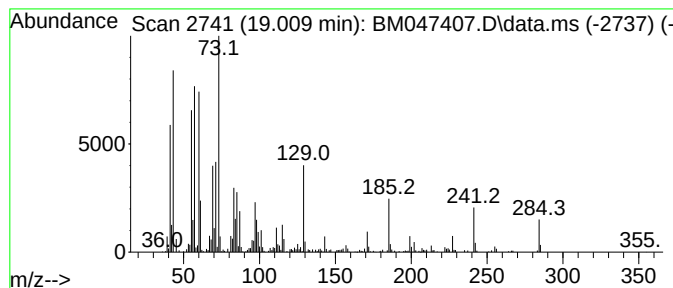
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.009	4.08 ng	459901	Chrysene-d12	21.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047407.D
Acq On : 30 Aug 2024 15:40
Operator : RC/JU
Sample : P3799-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TEST-PITS-4

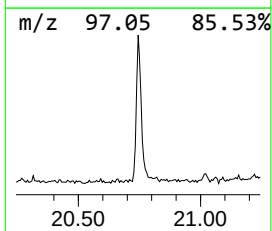
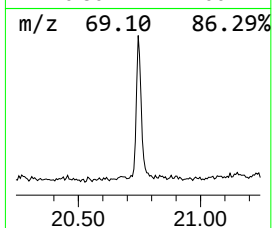
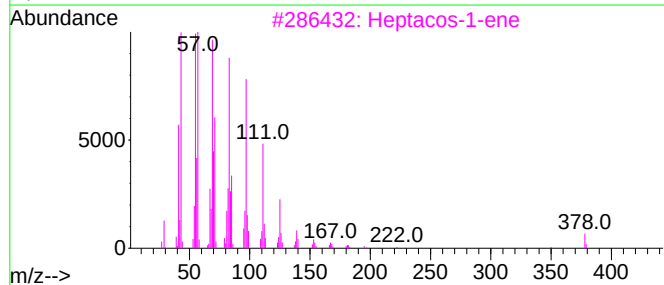
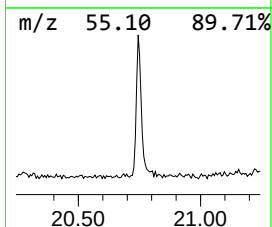
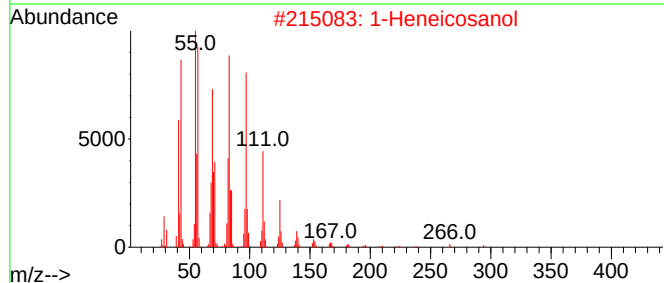
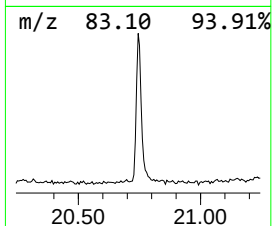
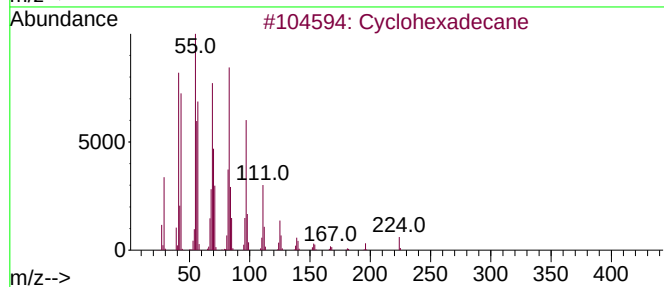
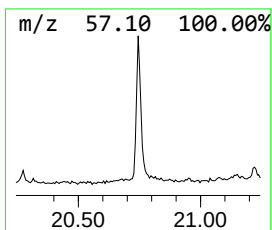
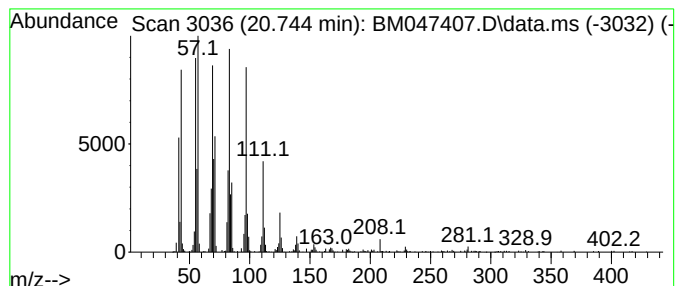
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.744	5.45 ng	613761	Chrysene-d12	21.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	94
2			1-Heneicosanol	312	C21H44O	015594-90-8	94
3			Heptacos-1-ene	378	C27H54	015306-27-1	94
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5			Pentacos-1-ene	350	C25H50	016980-85-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047407.D
Acq On : 30 Aug 2024 15:40
Operator : RC/JU
Sample : P3799-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TEST-PITS-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.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-...	4.557	5.1	ng	296974	1	7.345	1162760	20.0
Benzophenone	15.392	17.0	ng	2059370	4	16.774	2417120	20.0
Methanone, (1-h...	15.957	2.8	ng	335017	4	16.774	2417120	20.0
n-Hexadecanoic ...	17.709	11.3	ng	1362520	4	16.774	2417120	20.0
Octadecanoic acid	19.009	4.1	ng	459901	5	21.021	2251850	20.0
Cyclohexadecane	20.744	5.5	ng	613761	5	21.021	2251850	20.0