

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
 Data File : BM047260.D
 Acq On : 19 Aug 2024 20:09
 Operator : RC/JU
 Sample : P3637-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 ETGI - 370

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-BM081024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047260.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.257	60	63	80	rBV	123606	204381	1.90%	0.299%
2	4.569	280	286	293	rVB	143459	207201	1.92%	0.303%
3	5.016	356	362	374	rBV	2434945	3556698	33.04%	5.203%
4	6.575	621	627	638	rBV	2418731	3789266	35.20%	5.543%
5	7.363	753	761	768	rBV	824435	1259582	11.70%	1.842%
6	8.510	949	956	966	rBV	1572212	2542954	23.62%	3.720%
7	10.116	1221	1229	1236	rBV	1077641	1776517	16.50%	2.599%
8	10.880	1353	1359	1369	rBV	78550	155066	1.44%	0.227%
9	12.627	1648	1656	1671	rBV	4054359	5981363	55.56%	8.749%
10	13.904	1866	1873	1879	rBV3	48994	124132	1.15%	0.182%
11	14.021	1887	1893	1900	rBV	1713408	2468804	22.93%	3.611%
12	14.274	1934	1936	1942	rVB	90891	120854	1.12%	0.177%
13	15.533	2143	2150	2160	rBV	3808121	5439172	50.52%	7.956%
14	16.786	2358	2363	2368	rBV	2257738	3150548	29.26%	4.609%
15	16.827	2368	2370	2375	rVB	198728	229361	2.13%	0.336%
16	16.921	2382	2386	2393	rVB	89031	129129	1.20%	0.189%
17	17.727	2517	2523	2531	rBV	1170607	1792423	16.65%	2.622%
18	18.862	2711	2716	2720	rBV	664758	903769	8.39%	1.322%
19	19.021	2739	2743	2755	rBV	623844	1034874	9.61%	1.514%
20	19.233	2771	2779	2785	rBV	567210	916528	8.51%	1.341%
21	19.456	2811	2817	2827	rVB	8073989	9761352	90.67%	14.279%
22	20.762	3036	3039	3050	rVB3	604591	938032	8.71%	1.372%
23	20.968	3070	3074	3078	rBV	3057394	3386092	31.45%	4.953%
24	21.027	3078	3084	3088	rVV	2693080	3971954	36.89%	5.810%
25	21.068	3088	3091	3099	rVB	333321	504355	4.68%	0.738%
26	22.068	3255	3261	3267	rBV	7165025	10765801	100.00%	15.748%
27	23.727	3537	3543	3560	rVB	1397378	3253509	30.22%	4.759%

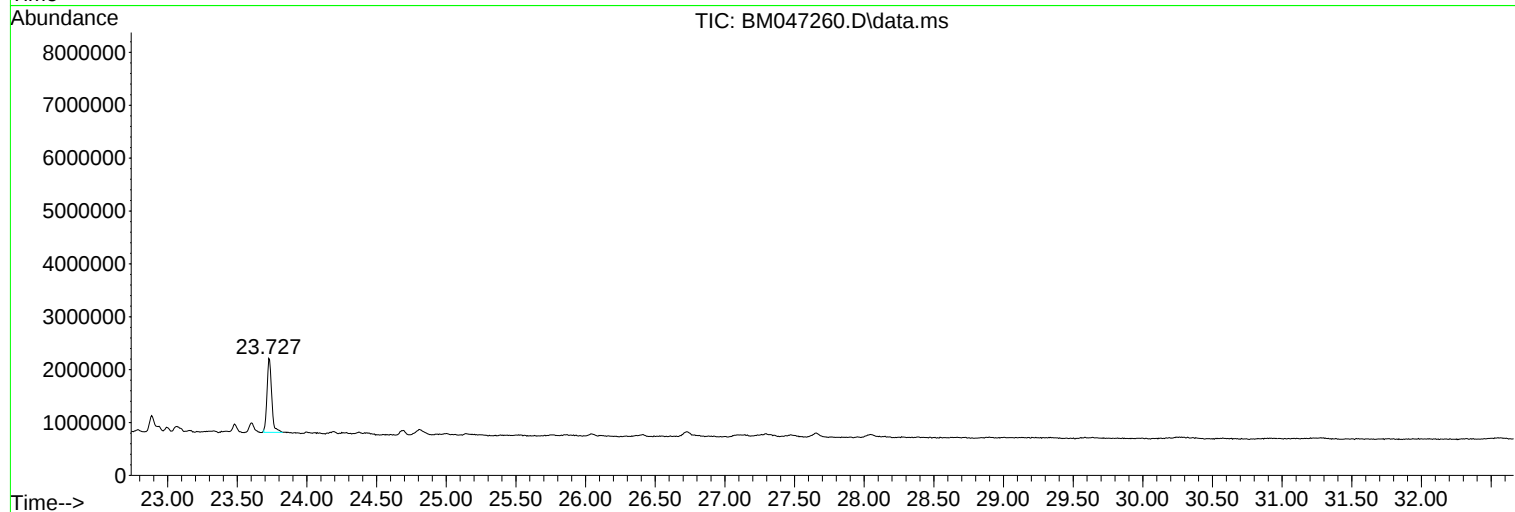
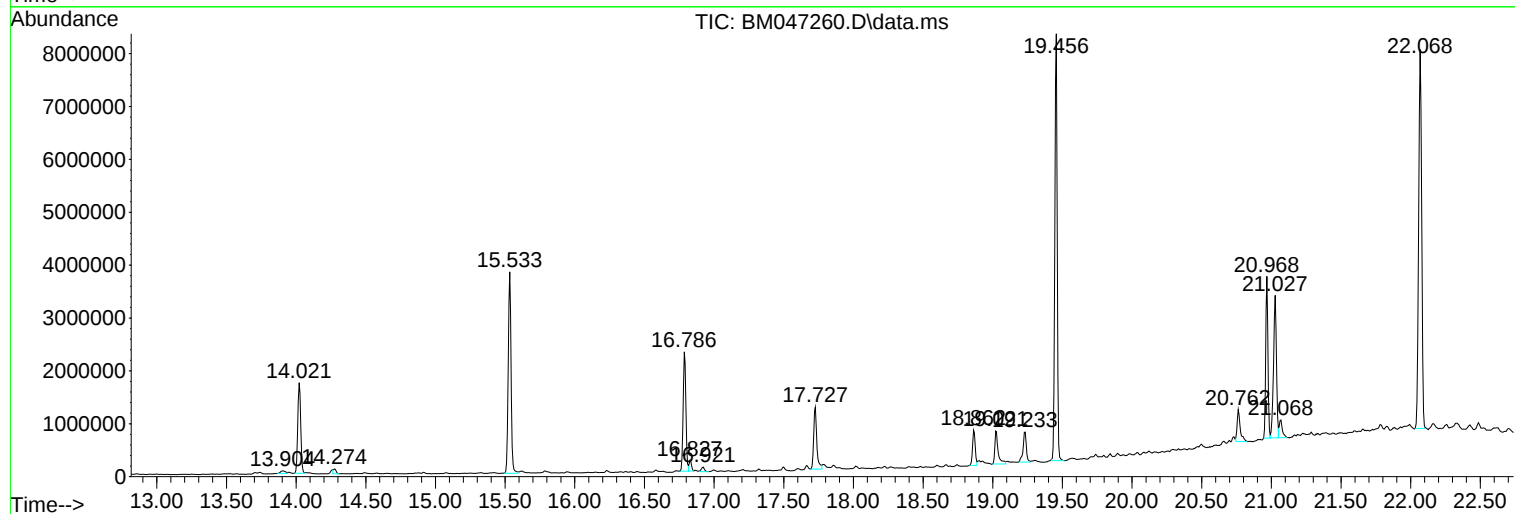
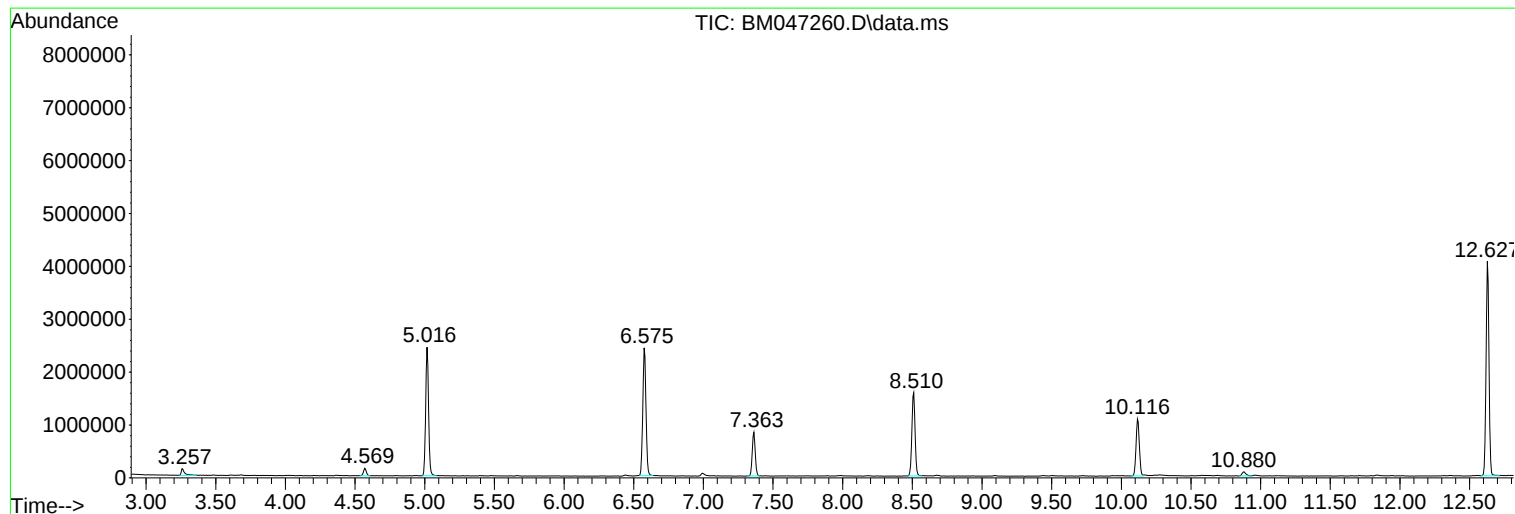
Sum of corrected areas: 68363717

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
Data File : BM047260.D
Acq On : 19 Aug 2024 20:09
Operator : RC/JU
Sample : P3637-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ETGI - 370

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.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\BM081924\
Data File : BM047260.D
Acq On : 19 Aug 2024 20:09
Operator : RC/JU
Sample : P3637-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ETGI - 370

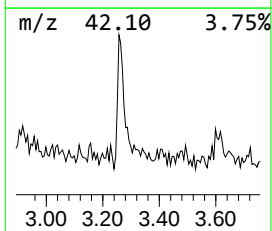
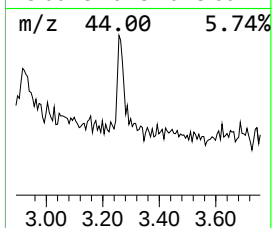
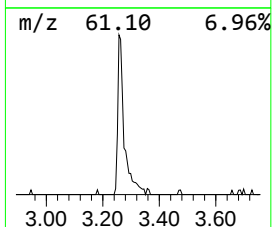
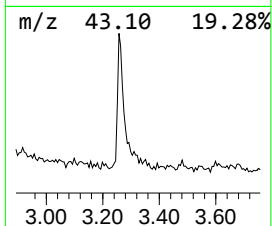
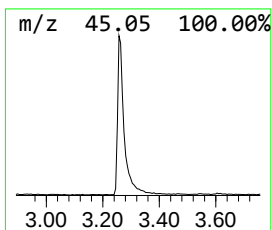
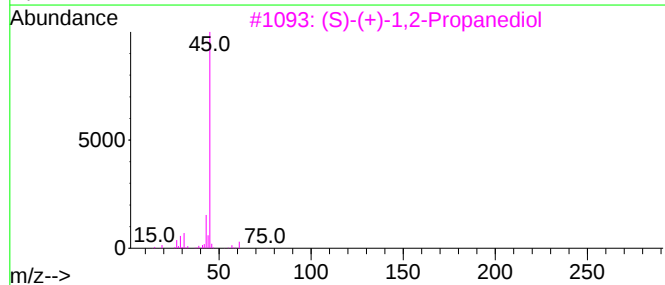
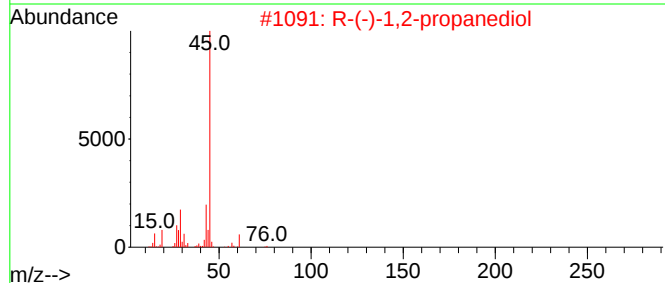
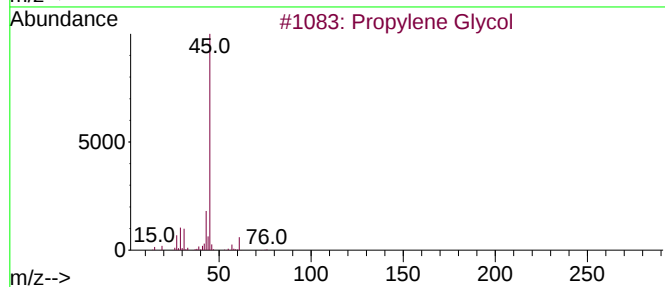
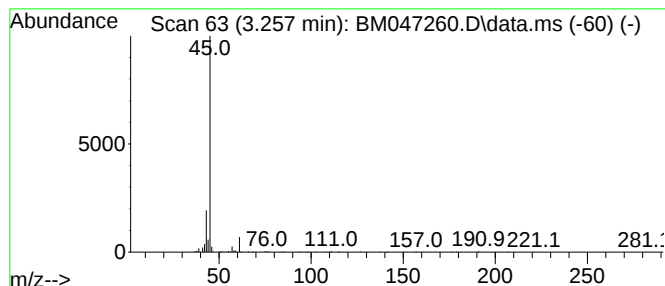
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propylene Glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.257	3.25 ng	204381	1,4-Dichlorobenzene-d4	7.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	86
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	72
3			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
4			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5			2-Pentanol	88	C5H12O	006032-29-7	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
Data File : BM047260.D
Acq On : 19 Aug 2024 20:09
Operator : RC/JU
Sample : P3637-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ETGI - 370

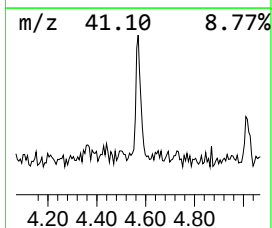
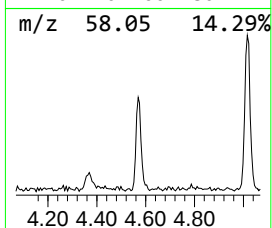
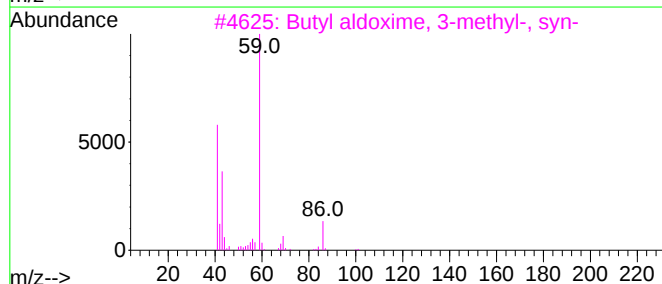
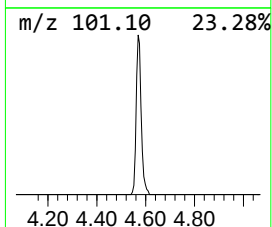
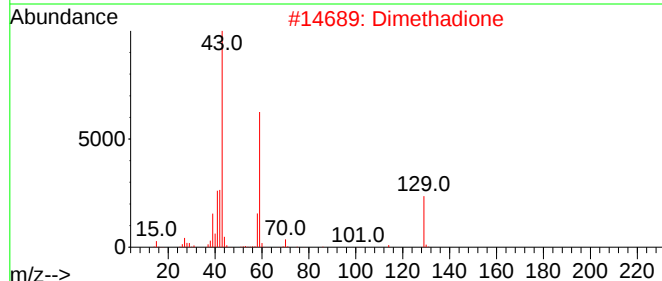
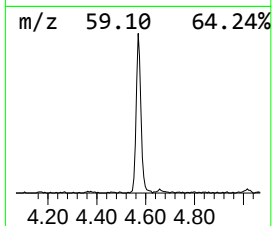
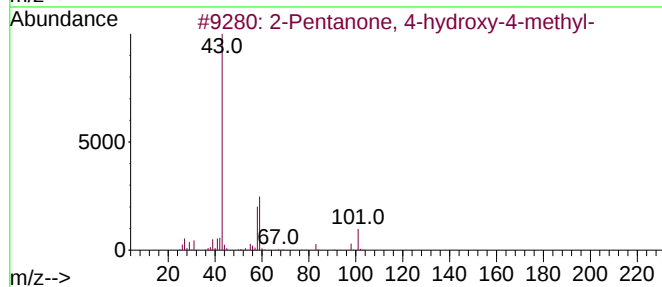
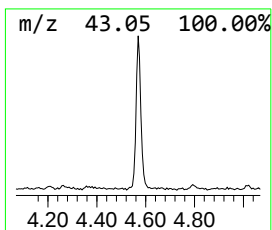
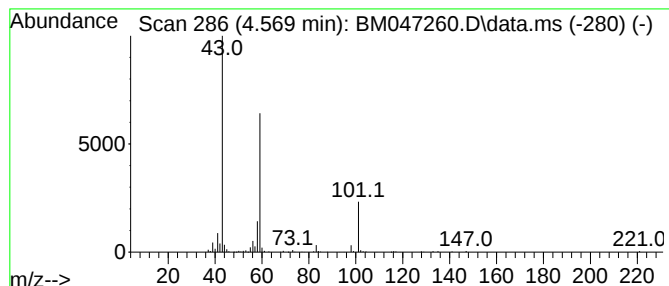
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.569	3.29 ng	207201	1,4-Dichlorobenzene-d4	7.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Dimethadione	129	C5H7NO3	000695-53-4	40		
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	38		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38		
5	3-Hexanol	102	C6H14O	000623-37-0	33		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
Data File : BM047260.D
Acq On : 19 Aug 2024 20:09
Operator : RC/JU
Sample : P3637-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ETGI - 370

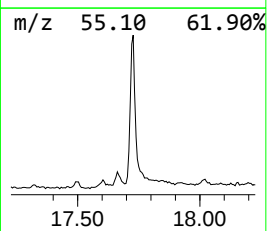
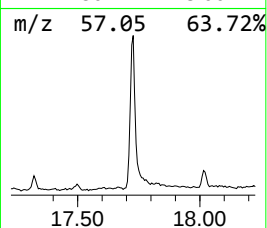
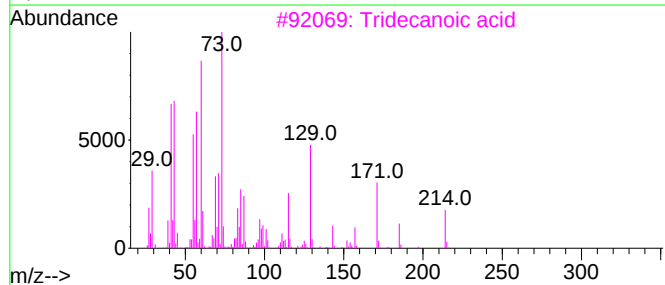
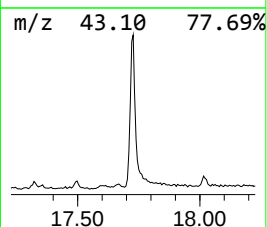
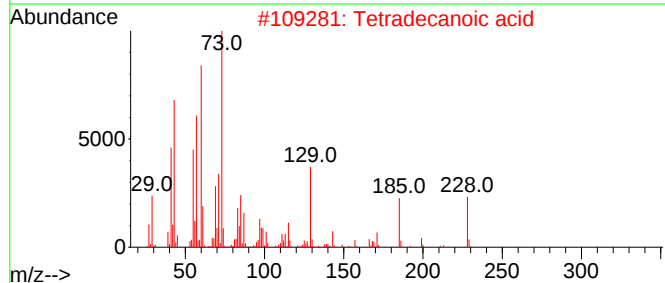
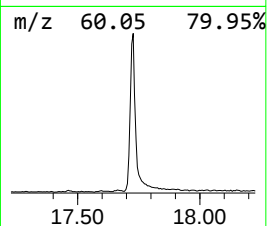
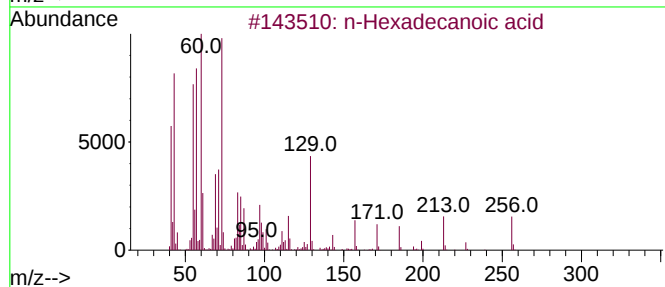
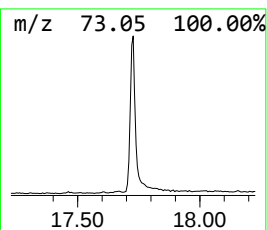
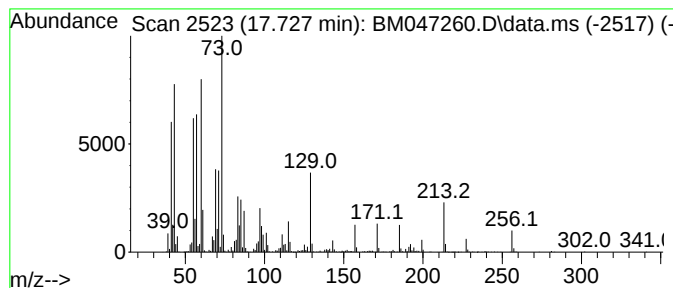
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.727	11.38 ng	1792420	Phenanthrene-d10	16.786

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	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	92
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5			n-Decanoic acid	172	C10H20O2	000334-48-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
Data File : BM047260.D
Acq On : 19 Aug 2024 20:09
Operator : RC/JU
Sample : P3637-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ETGI - 370

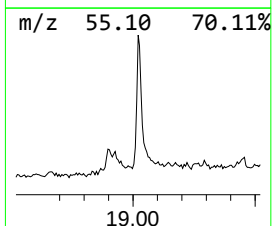
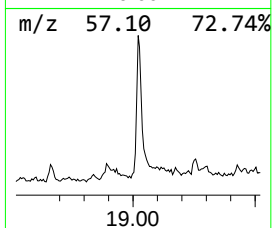
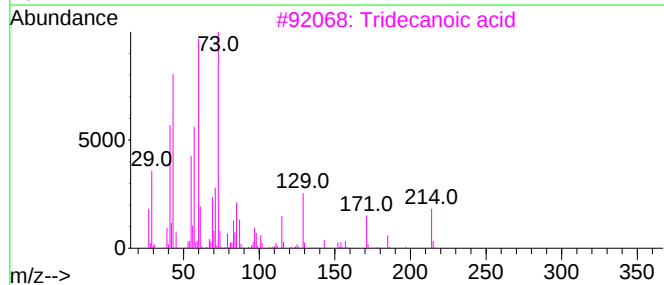
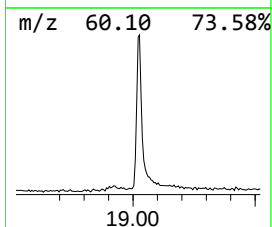
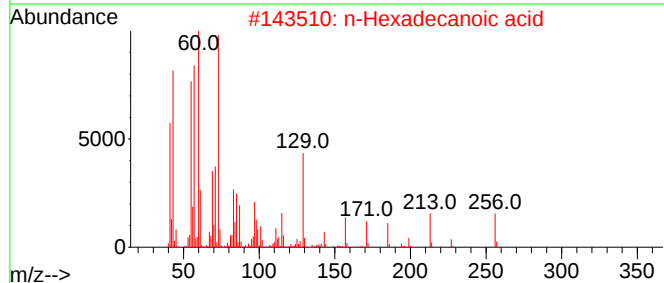
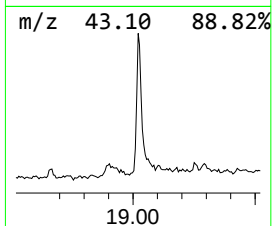
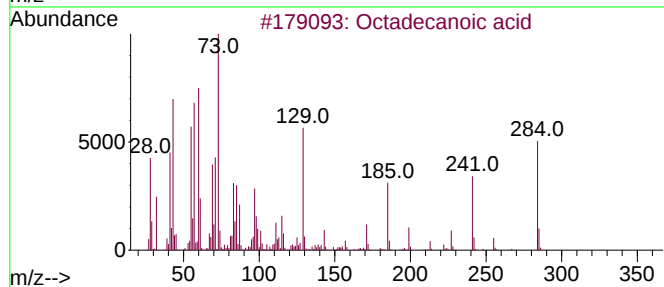
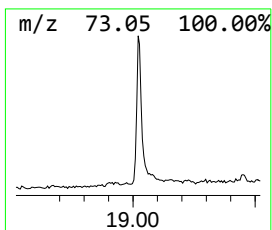
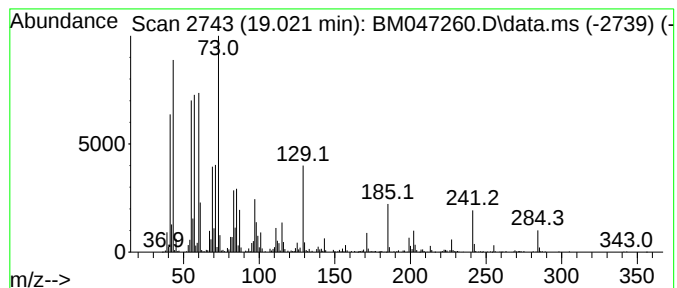
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.021	5.21 ng	1034870	Chrysene-d12	21.027

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	83
3			Tridecanoic acid	214	C13H26O2	000638-53-9	81
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
Data File : BM047260.D
Acq On : 19 Aug 2024 20:09
Operator : RC/JU
Sample : P3637-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ETGI - 370

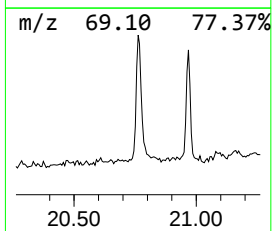
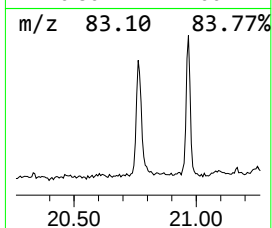
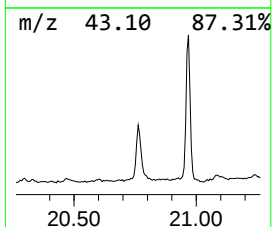
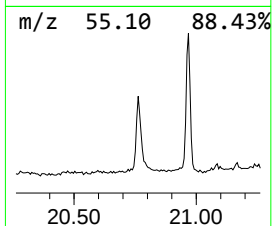
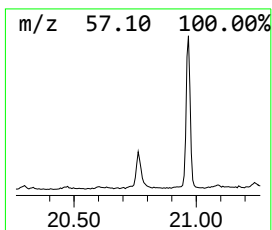
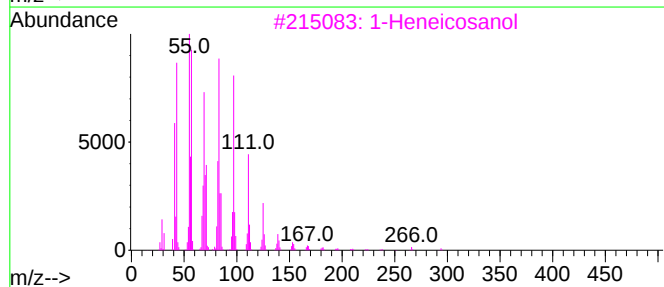
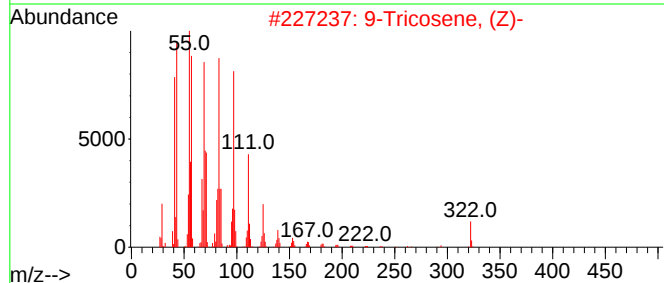
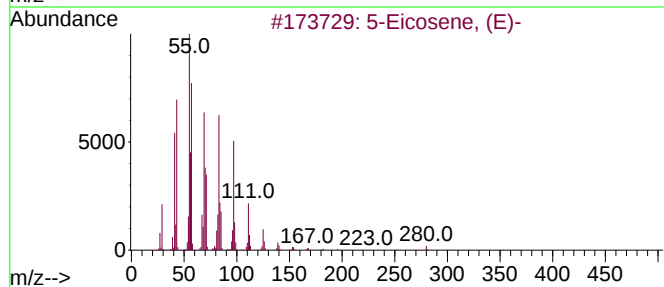
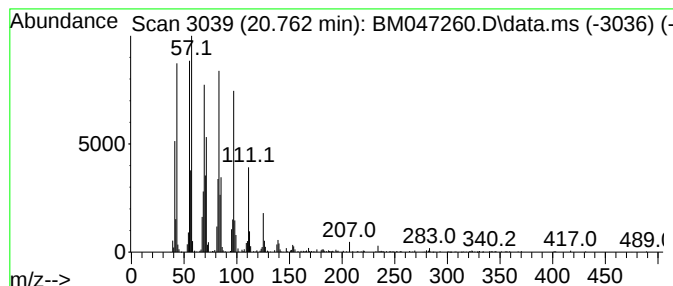
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.762	4.72 ng	938032	Chrysene-d12	21.027

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2		9-Tricosene, (Z)-	322	C23H46	027519-02-4	95
3		1-Heneicosanol	312	C21H44O	015594-90-8	95
4		Heptacos-1-ene	378	C27H54	015306-27-1	94
5		1-Tetracosene	336	C24H48	010192-32-2	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
Data File : BM047260.D
Acq On : 19 Aug 2024 20:09
Operator : RC/JU
Sample : P3637-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ETGI - 370

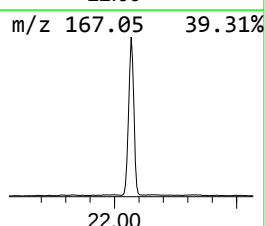
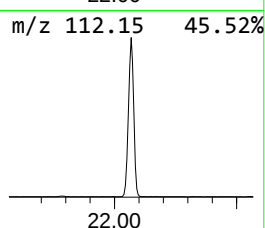
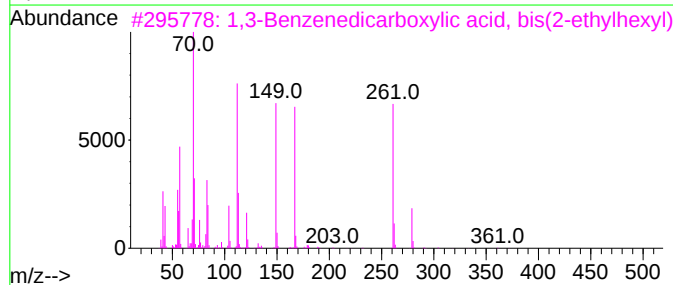
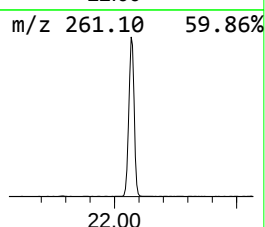
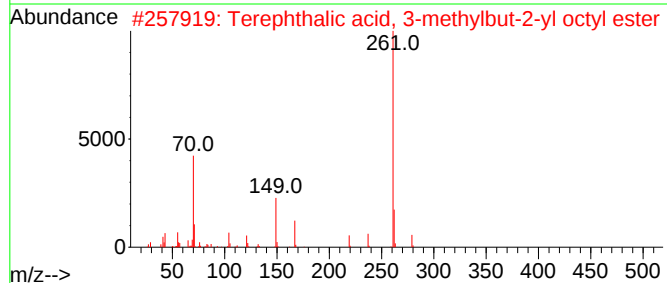
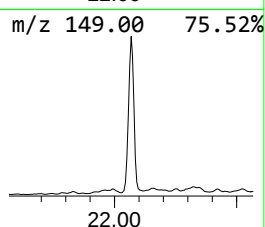
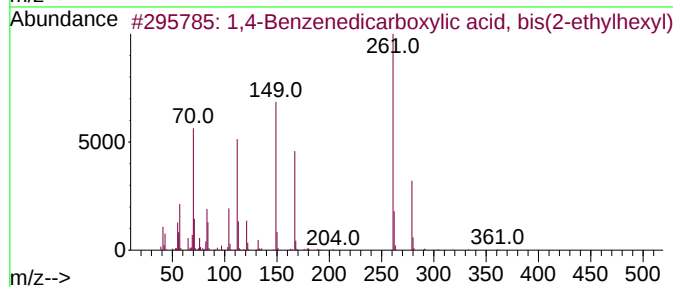
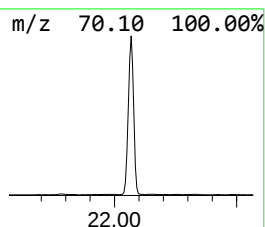
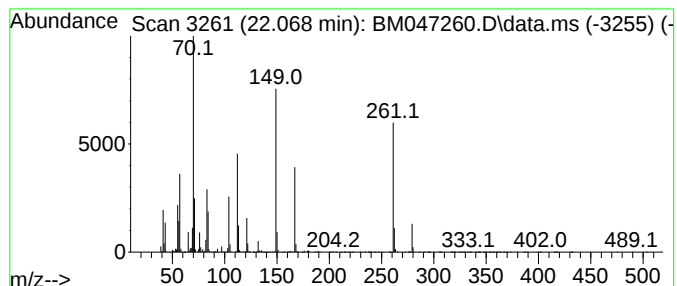
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,4-Benzenedicarboxylic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.068	54.21 ng	10765800	Chrysene-d12	21.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H3804	006422-86-2	87
2			Terephthalic acid, 3-methylbut-2...	348	C21H3204	1000356-27-6	58
3			1,3-Benzenedicarboxylic acid, bi...	390	C24H3804	000137-89-3	49
4			Isophthalic acid, 3-methylbut-2...	348	C21H3204	1000344-72-4	47
5			Terephthalic acid, 2-ethylhexyl ...	390	C24H3804	1000324-00-5	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
Data File : BM047260.D
Acq On : 19 Aug 2024 20:09
Operator : RC/JU
Sample : P3637-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ETGI - 370

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.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
Propylene Glycol	3.257	3.3	ng	204381	1	7.363	1259580	20.0
2-Pentanone, 4-...	4.569	3.3	ng	207201	1	7.363	1259580	20.0
n-Hexadecanoic ...	17.727	11.4	ng	1792420	4	16.786	3150550	20.0
Octadecanoic acid	19.021	5.2	ng	1034870	5	21.027	3971950	20.0
5-Eicosene, (E)-	20.762	4.7	ng	938032	5	21.027	3971950	20.0
1,4-Benzenedica...	22.068	54.2	ng	10765800	5	21.027	3971950	20.0