

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050724\
 Data File : BF137846.D
 Acq On : 07 May 2024 14:37
 Operator : CG\JU
 Sample : P2312-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-125-SB-02

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_F\Methods\8270-BF043024.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137846.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	10	21	28	rVB	43477	120226	2.31%	0.346%
2	2.440	51	60	66	rVB	2037862	2817347	54.20%	8.118%
3	5.681	605	611	614	rBV	3629988	3768197	72.49%	10.858%
4	6.669	772	779	781	rBV	3004890	3827515	73.64%	11.029%
5	7.051	840	844	847	rVB	1053351	865566	16.65%	2.494%
6	7.616	934	940	947	rBV	2349095	2601587	50.05%	7.496%
7	8.298	1052	1056	1058	rBV	108688	83776	1.61%	0.241%
8	8.334	1058	1062	1065	rVV	1473513	1172614	22.56%	3.379%
9	8.910	1156	1160	1164	rVB	233783	192716	3.71%	0.555%
10	9.410	1240	1245	1248	rBV	5566358	5197889	100.00%	14.978%
11	9.475	1253	1256	1259	rVB	168462	126481	2.43%	0.364%
12	10.098	1357	1362	1365	rBV	1592036	1437311	27.65%	4.142%
13	10.181	1372	1376	1383	rBV2	67868	91762	1.77%	0.264%
14	10.892	1492	1497	1500	rBV	3560497	3320196	63.88%	9.567%
15	11.592	1612	1616	1619	rBV	1698166	1366923	26.30%	3.939%
16	12.104	1697	1703	1719	rBV	769572	824142	15.86%	2.375%
17	12.804	1816	1822	1828	rBV5	41389	78751	1.52%	0.227%
18	12.886	1832	1836	1848	rVV	224466	233843	4.50%	0.674%
19	12.975	1848	1851	1857	rVB	130763	109371	2.10%	0.315%
20	13.180	1881	1886	1889	rBV	4728913	4364878	83.97%	12.577%
21	13.704	1972	1975	1978	rBV	118379	107722	2.07%	0.310%
22	14.139	2040	2049	2052	rBV7	31925	98959	1.90%	0.285%
23	14.239	2063	2066	2070	rBV	972247	881228	16.95%	2.539%
24	14.380	2086	2090	2097	rBV	54239	55600	1.07%	0.160%
25	15.110	2210	2214	2219	rBV	132591	140880	2.71%	0.406%
26	15.815	2328	2334	2345	rBV	628134	818590	15.75%	2.359%

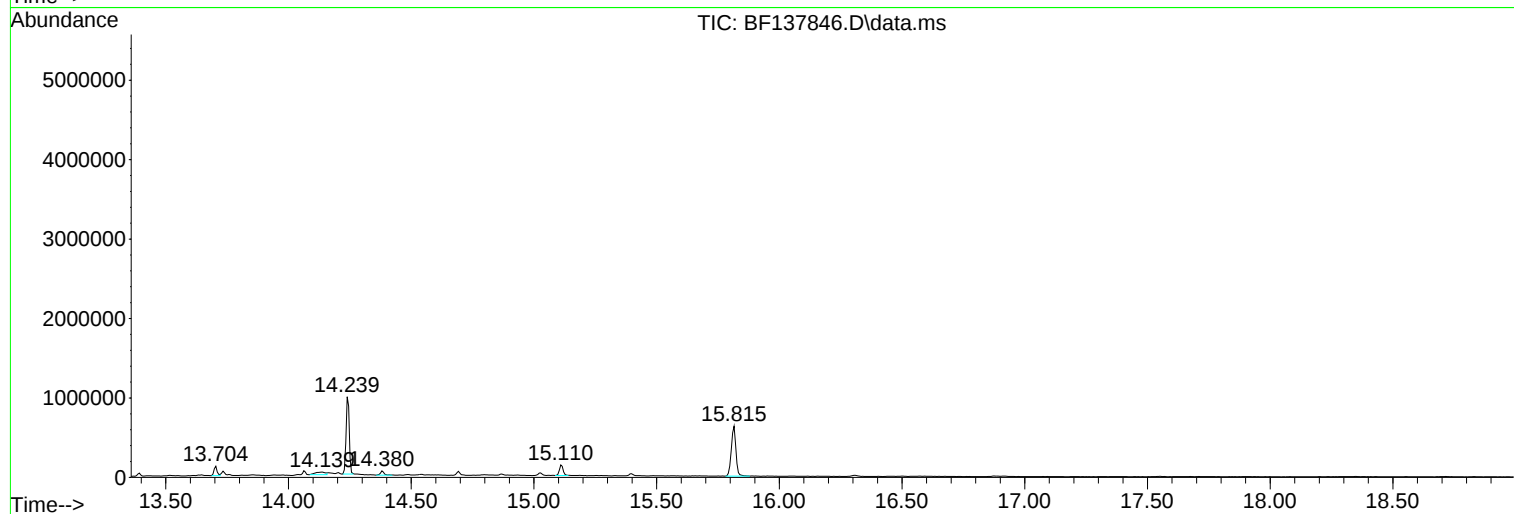
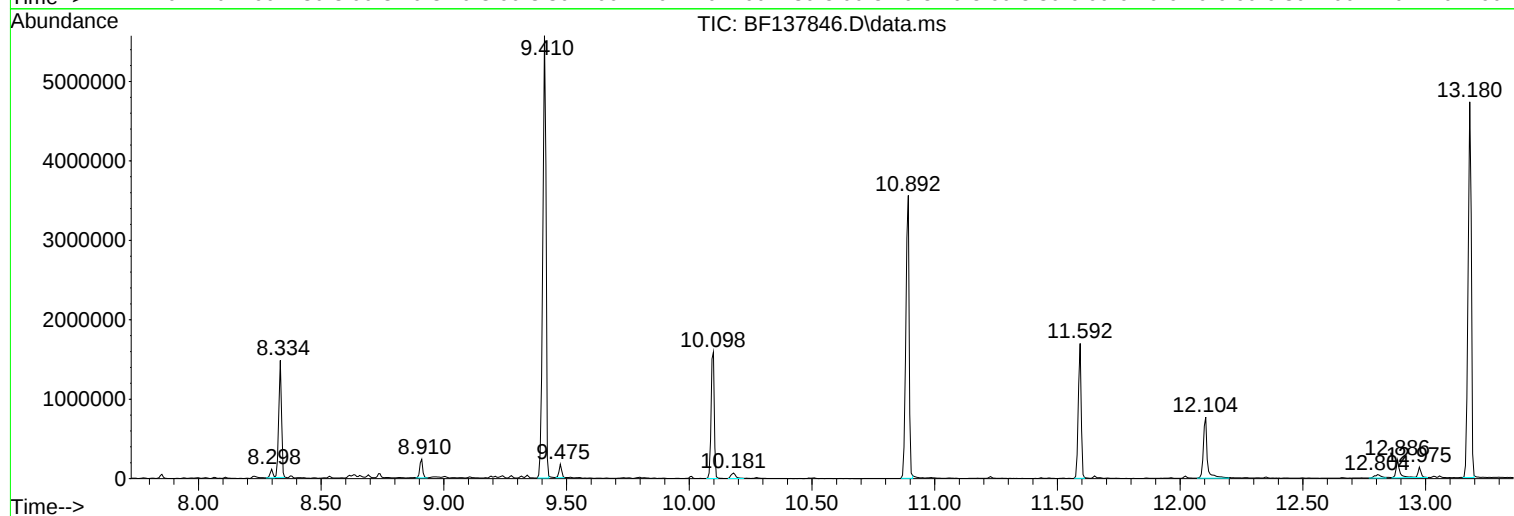
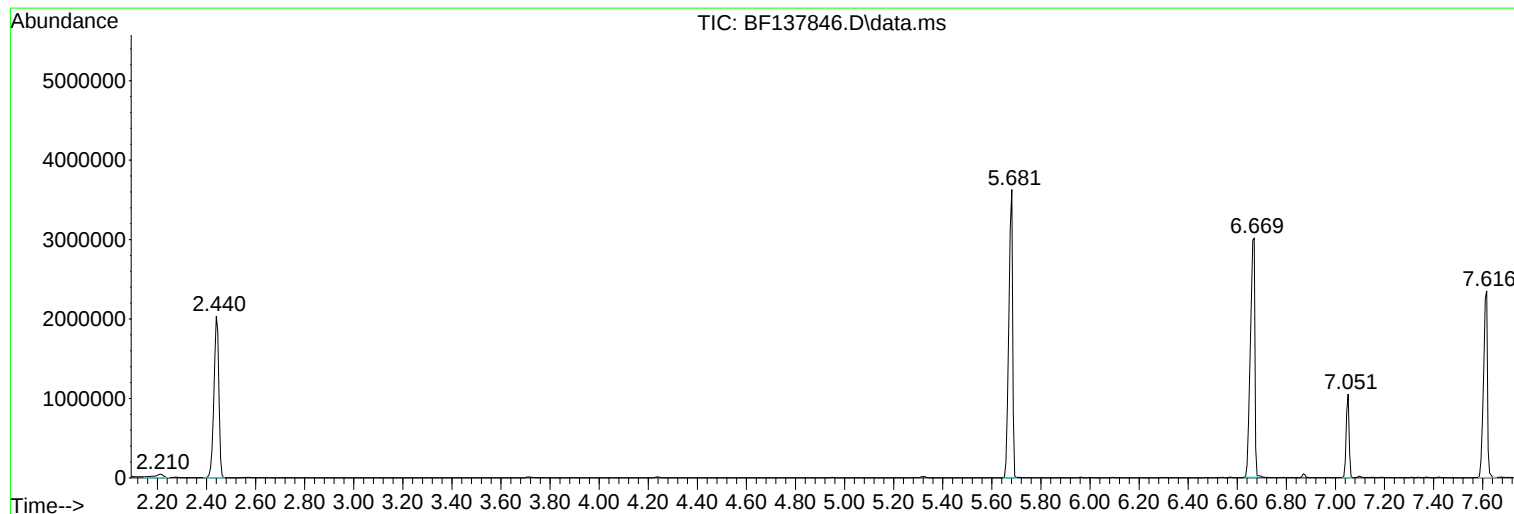
Sum of corrected areas: 34704070

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050724\
Data File : BF137846.D
Acq On : 07 May 2024 14:37
Operator : CG\JU
Sample : P2312-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-125-SB-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.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_F\Data\BF050724\
Data File : BF137846.D
Acq On : 07 May 2024 14:37
Operator : CG\JU
Sample : P2312-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-125-SB-02

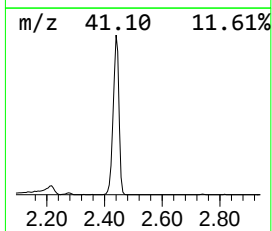
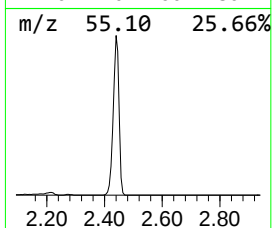
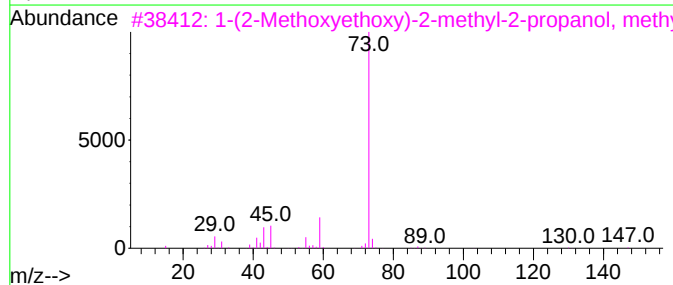
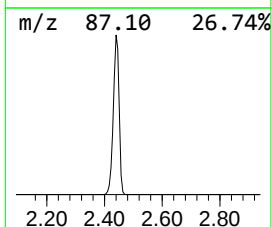
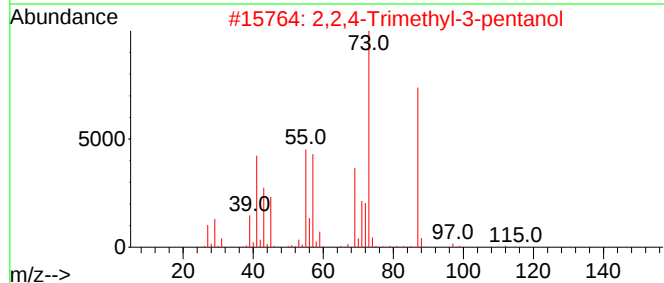
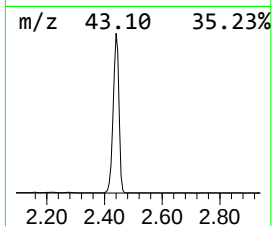
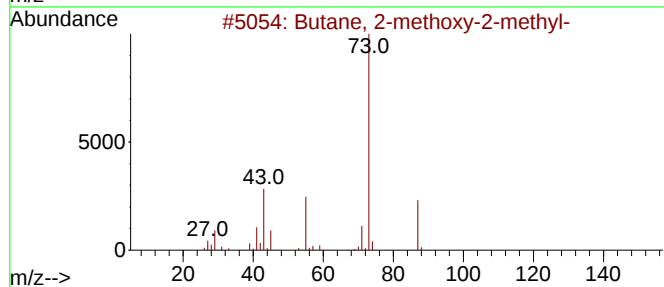
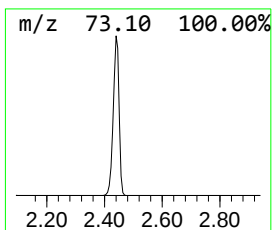
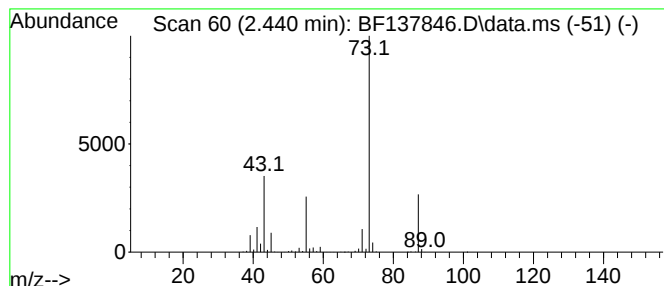
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.440	65.10 ng	2817350	1,4-Dichlorobenzene-d4	7.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050724\
Data File : BF137846.D
Acq On : 07 May 2024 14:37
Operator : CG\JU
Sample : P2312-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-125-SB-02

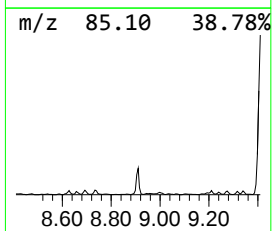
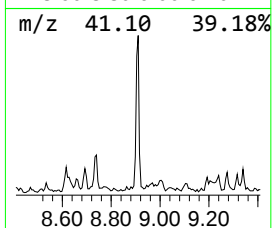
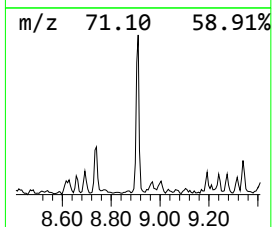
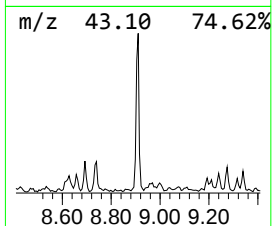
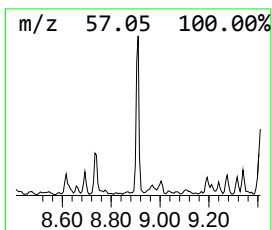
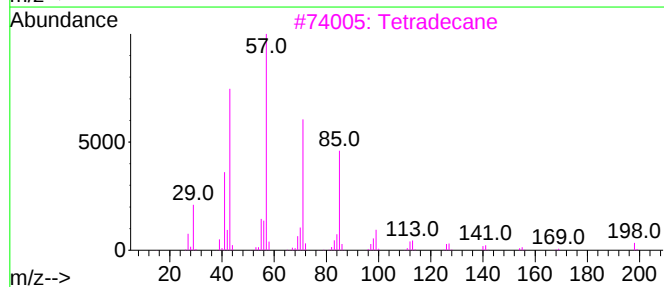
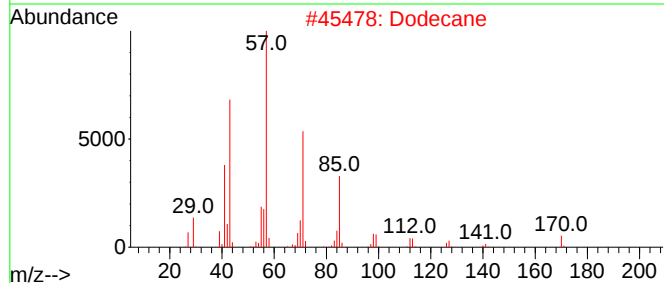
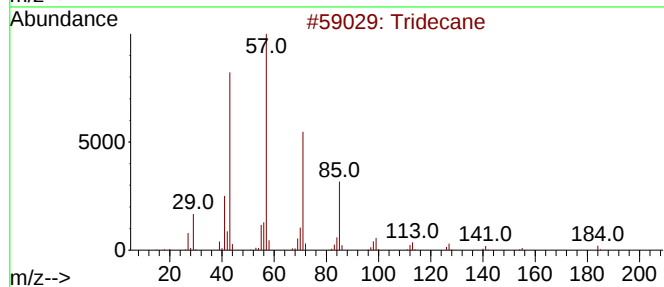
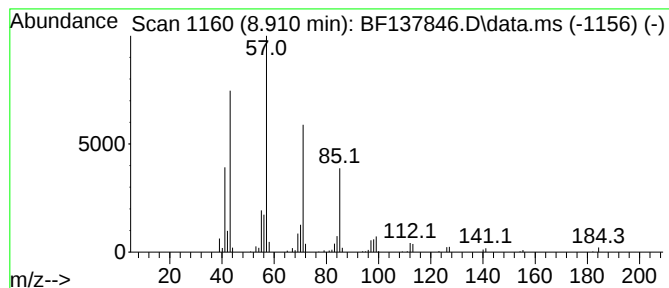
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Tridecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.910	3.29 ng	192716	Naphthalene-d8	8.334

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecane	184	C13H28	000629-50-5	97
2		Dodecane	170	C12H26	000112-40-3	90
3		Tetradecane	198	C14H30	000629-59-4	90
4		Hexadecane	226	C16H34	000544-76-3	87
5		Nonadecane	268	C19H40	000629-92-5	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050724\
Data File : BF137846.D
Acq On : 07 May 2024 14:37
Operator : CG\JU
Sample : P2312-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-125-SB-02

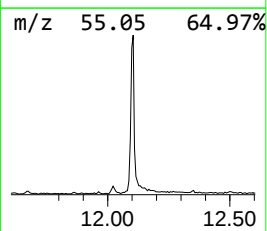
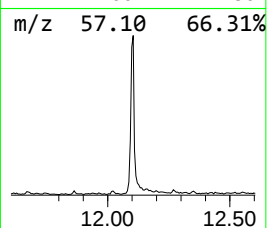
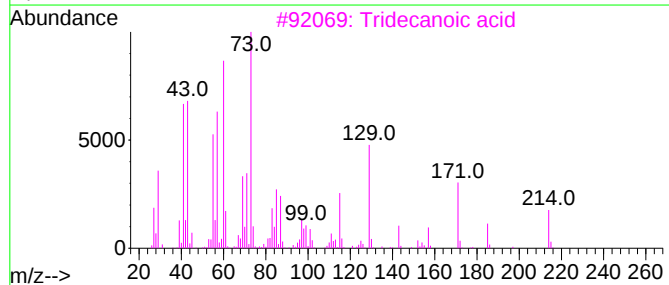
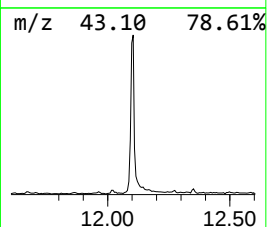
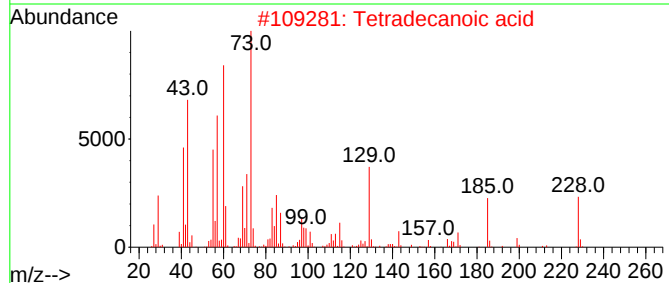
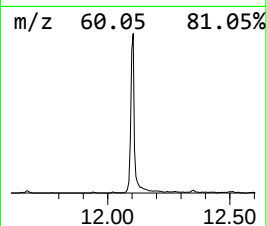
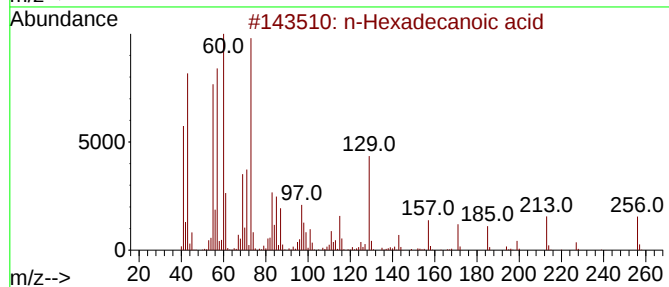
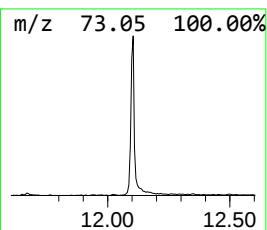
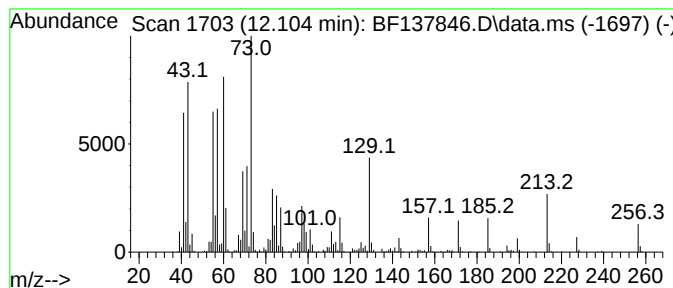
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
12.104	12.06 ng	824142	Phenanthrene-d10	11.592

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	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			Undecanoic acid	186	C11H22O2	000112-37-8	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050724\
Data File : BF137846.D
Acq On : 07 May 2024 14:37
Operator : CG\JU
Sample : P2312-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-125-SB-02

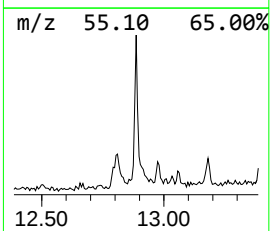
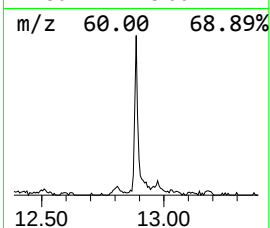
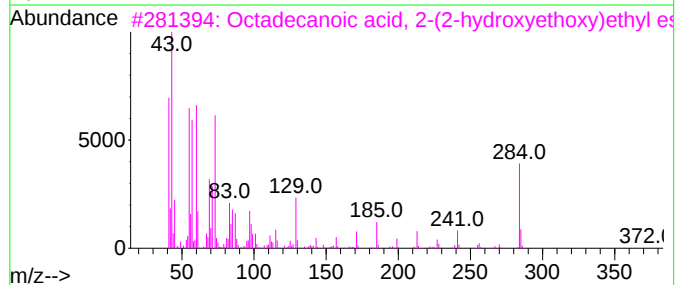
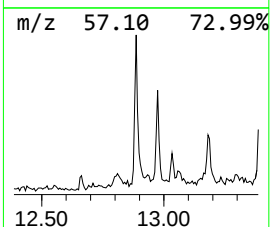
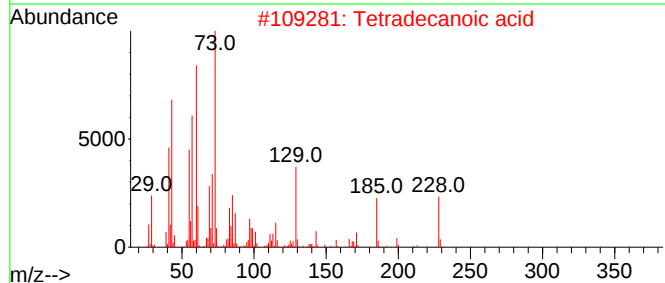
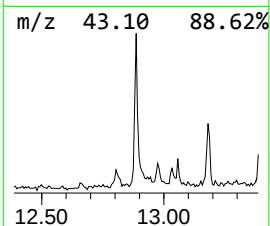
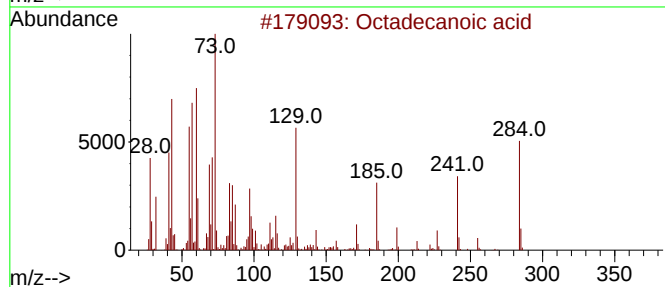
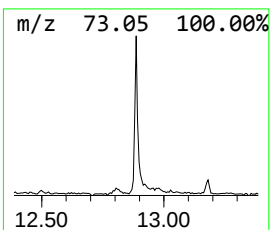
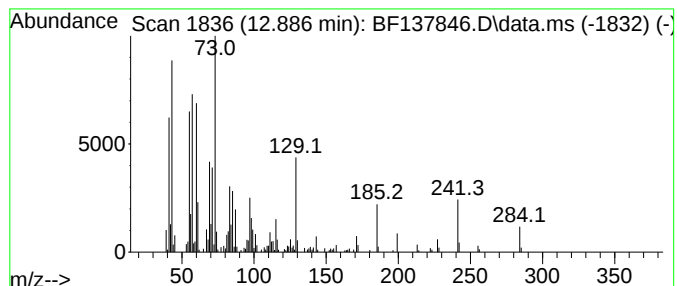
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.886	3.42 ng	233843	Phenanthrene-d10	11.592

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050724\
Data File : BF137846.D
Acq On : 07 May 2024 14:37
Operator : CG\JU
Sample : P2312-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-125-SB-02

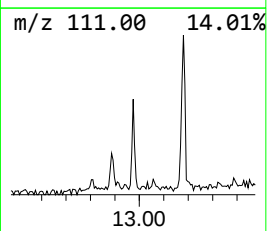
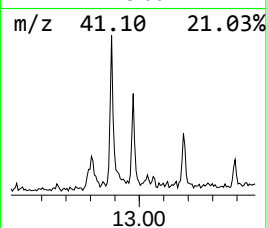
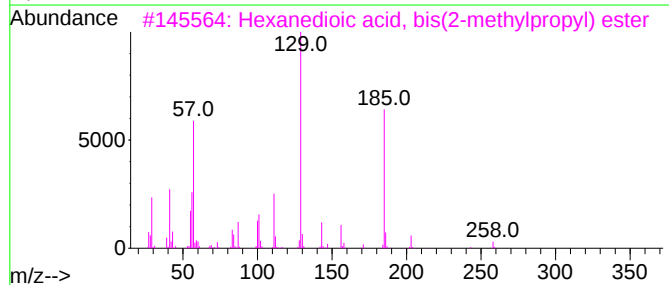
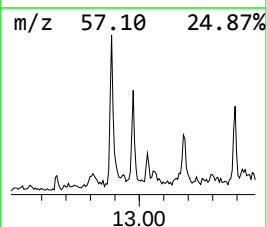
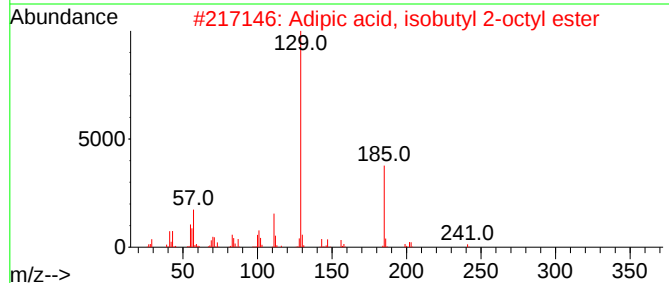
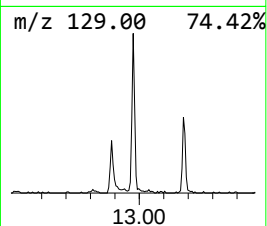
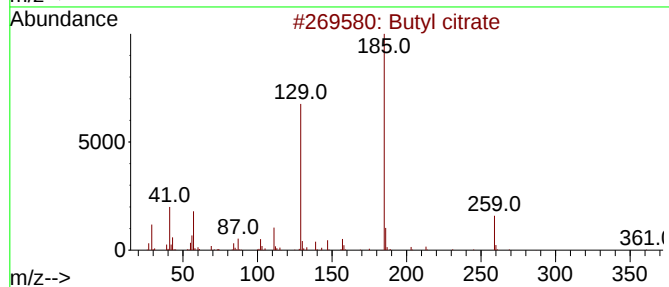
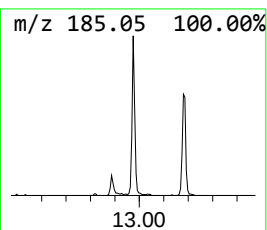
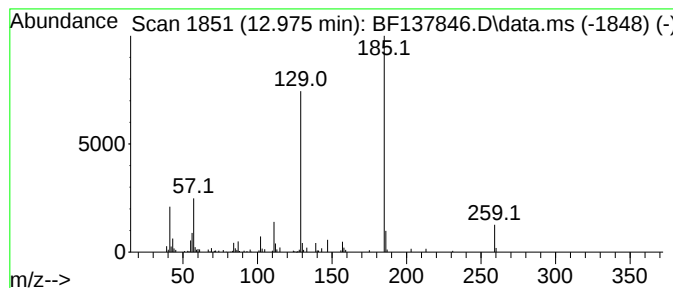
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Butyl citrate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.975	2.48 ng	109371	Chrysene-d12	14.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl citrate	360	C18H32O7	000077-94-1	91
2			Adipic acid, isobutyl 2-octyl ester	314	C18H34O4	1000324-44-5	78
3			Hexanedioic acid, bis(2-methylpr...	258	C14H26O4	000141-04-8	72
4			Adipic acid, butyl 3-pentyl ester	272	C15H28O4	1000324-60-5	64
5			Adipic acid, isobutyl 2-pentyl e...	272	C15H28O4	1000324-15-6	56



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050724\
Data File : BF137846.D
Acq On : 07 May 2024 14:37
Operator : CG\JU
Sample : P2312-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-125-SB-02

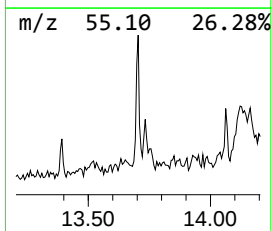
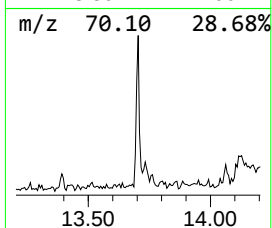
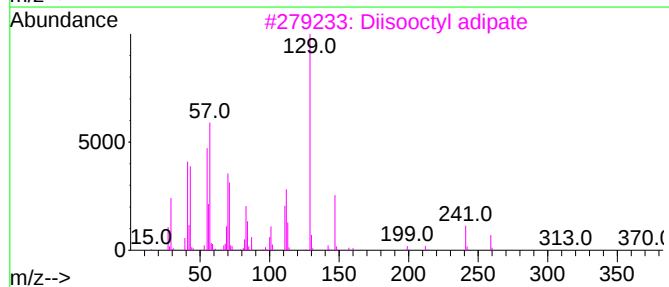
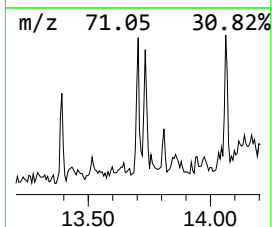
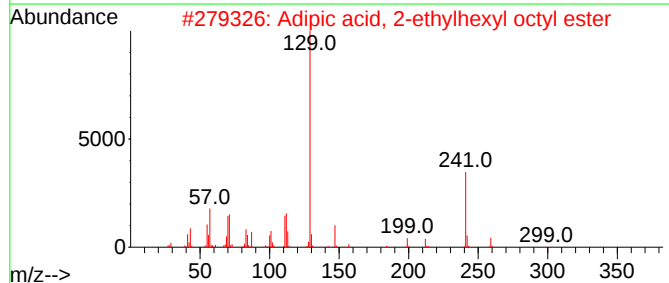
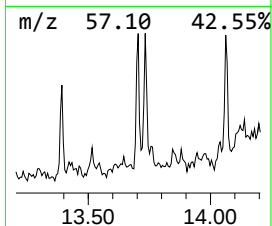
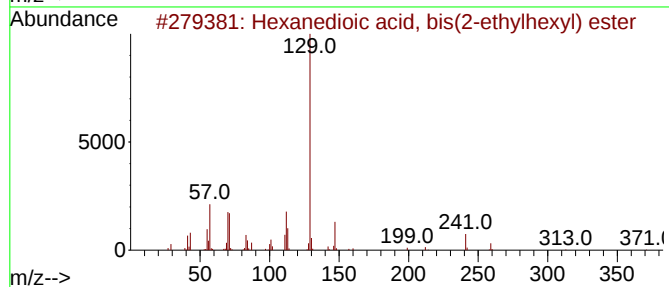
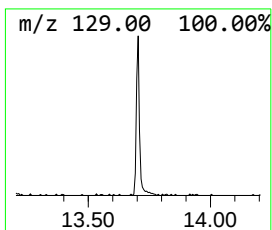
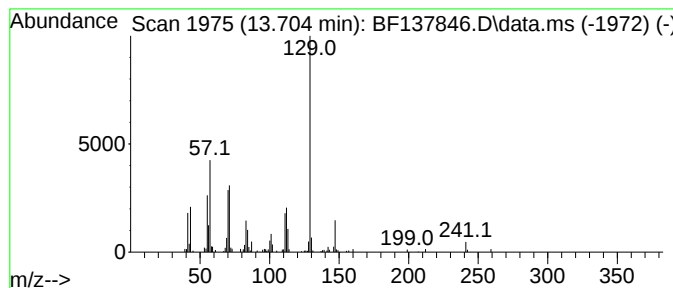
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexanedioic acid, bis(2-eth... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.704	2.44 ng	107722	Chrysene-d12	14.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	91
2			Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	90
3			Diisooctyl adipate	370	C22H42O4	001330-86-5	78
4			Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	76
5			Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1010324-48-0	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050724\
Data File : BF137846.D
Acq On : 07 May 2024 14:37
Operator : CG\JU
Sample : P2312-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-125-SB-02

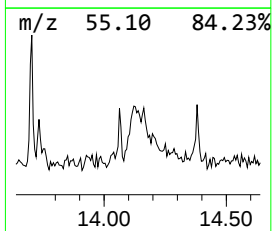
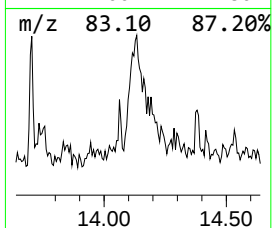
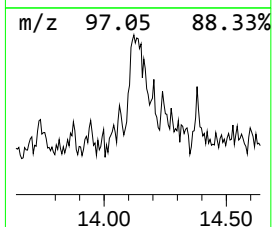
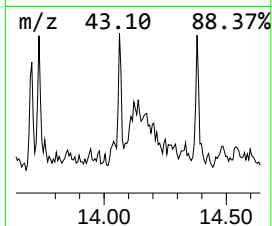
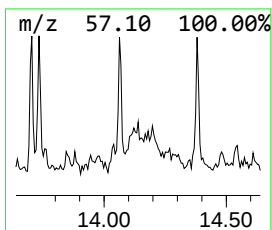
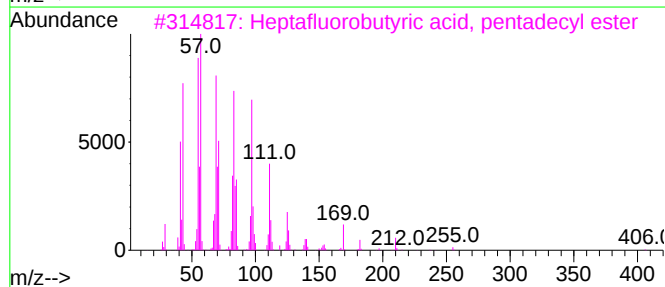
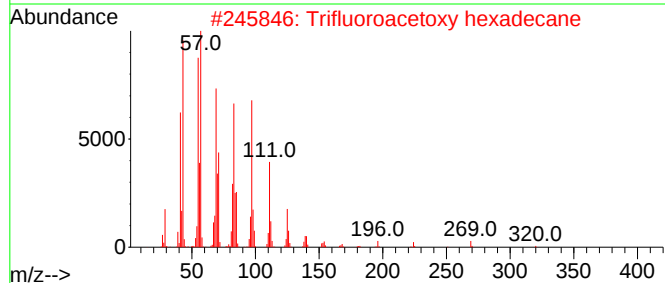
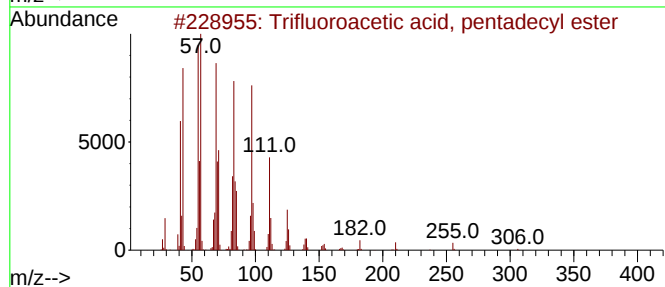
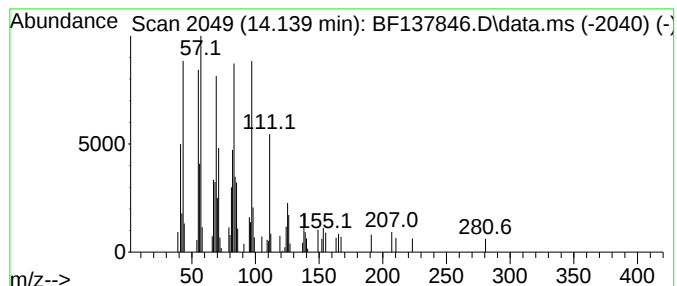
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Trifluoroacetic acid, penta... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.139	2.25 ng	98959	Chrysene-d12	14.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
5			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050724\
Data File : BF137846.D
Acq On : 07 May 2024 14:37
Operator : CG\JU
Sample : P2312-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-125-SB-02

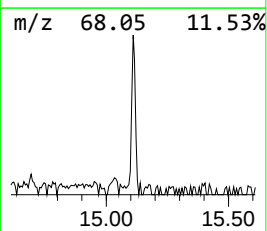
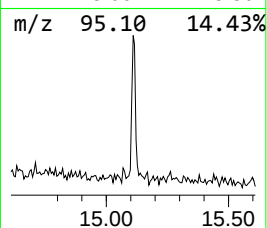
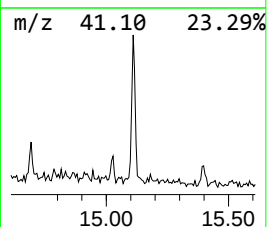
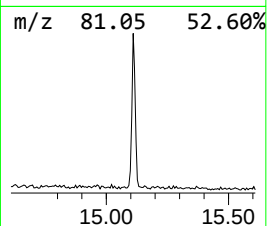
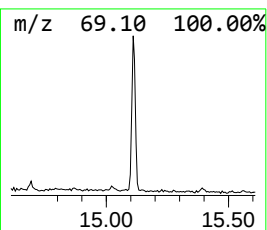
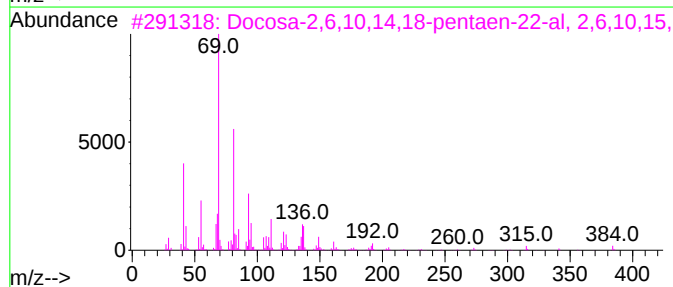
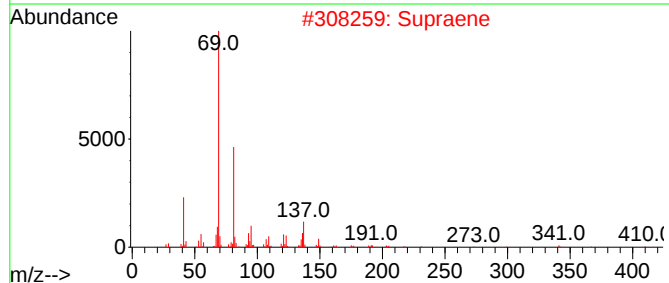
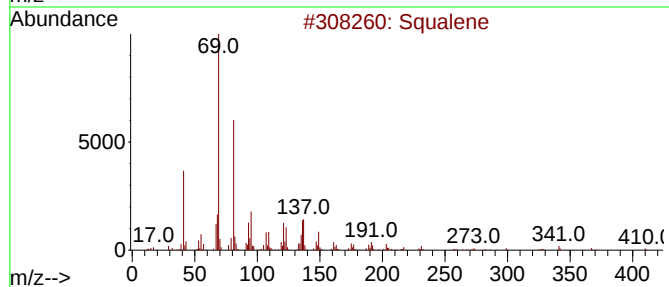
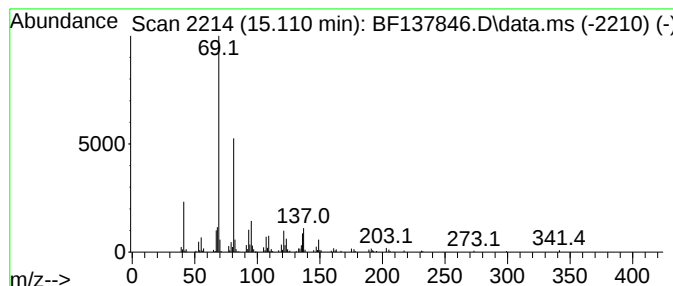
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.110	3.44 ng	140880	Perylene-d12	15.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	91
2			Supraene	410	C30H50	007683-64-9	91
3			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
4			3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	59
5			4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050724\
Data File : BF137846.D
Acq On : 07 May 2024 14:37
Operator : CG\JU
Sample : P2312-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-125-SB-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.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
Butane, 2-metho...	2.440	65.1	ng	2817350	1	7.051	865566	20.0
Tridecane	8.910	3.3	ng	192716	2	8.334	1172610	20.0
n-Hexadecanoic ...	12.104	12.1	ng	824142	4	11.592	1366920	20.0
Octadecanoic acid	12.886	3.4	ng	233843	4	11.592	1366920	20.0
Butyl citrate	12.975	2.5	ng	109371	5	14.239	881228	20.0
Hexanedioic aci...	13.704	2.4	ng	107722	5	14.239	881228	20.0
Trifluoroacetic...	14.139	2.3	ng	98959	5	14.239	881228	20.0
Squalene	15.110	3.4	ng	140880	6	15.816	818590	20.0