

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030424\
 Data File : BF137482.D
 Acq On : 04 Mar 2024 15:49
 Operator : CG\JU
 Sample : P1662-03
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RBR-2520556

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-BF022924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137482.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	10	17	26	rVB	1371008	1806452	38.50%	4.938%
2	5.122	513	516	525	rBV	49252	68357	1.46%	0.187%
3	5.510	578	582	604	rBV	4352649	4124048	87.89%	11.273%
4	6.498	745	750	771	rBV	4028920	4355554	92.82%	11.906%
5	6.857	807	811	829	rBV	1388327	1286553	27.42%	3.517%
6	7.416	902	906	920	rBV	2748754	2721692	58.00%	7.440%
7	8.127	1024	1027	1048	rBV	1890098	1750639	37.31%	4.785%
8	9.210	1206	1211	1214	rBV	5396114	4692246	100.00%	12.827%
9	9.886	1322	1326	1330	rBV	2461651	2000147	42.63%	5.468%
10	9.992	1339	1344	1352	rVB	71156	98721	2.10%	0.270%
11	10.680	1457	1461	1480	rBV	3069321	2812872	59.95%	7.689%
12	11.380	1577	1580	1583	rBV	2367535	1985885	42.32%	5.429%
13	11.933	1670	1674	1683	rBV2	271605	406557	8.66%	1.111%
14	12.604	1784	1788	1793	rBV	208147	205243	4.37%	0.561%
15	12.833	1821	1827	1831	rBV	192897	197558	4.21%	0.540%
16	12.986	1849	1853	1856	rBV	4826063	4369236	93.12%	11.944%
17	13.904	2005	2009	2018	rBV2	195837	295227	6.29%	0.807%
18	14.045	2028	2033	2036	rBV	1299333	1359512	28.97%	3.716%
19	14.698	2141	2144	2150	rBV	70351	87538	1.87%	0.239%
20	14.939	2181	2185	2191	rVB	116021	129862	2.77%	0.355%
21	15.115	2211	2215	2219	rBV	71498	114197	2.43%	0.312%
22	15.227	2230	2234	2237	rVB2	51782	60115	1.28%	0.164%
23	15.439	2266	2270	2275	rVB	39761	60784	1.30%	0.166%
24	15.504	2277	2281	2286	rBV	42302	59409	1.27%	0.162%
25	15.568	2287	2292	2301	rBV	877051	1196395	25.50%	3.270%
26	16.121	2379	2386	2393	rBV2	60254	123096	2.62%	0.336%
27	17.356	2589	2596	2603	rBV4	30446	85483	1.82%	0.234%
28	18.433	2772	2779	2787	rVB10	47847	128979	2.75%	0.353%

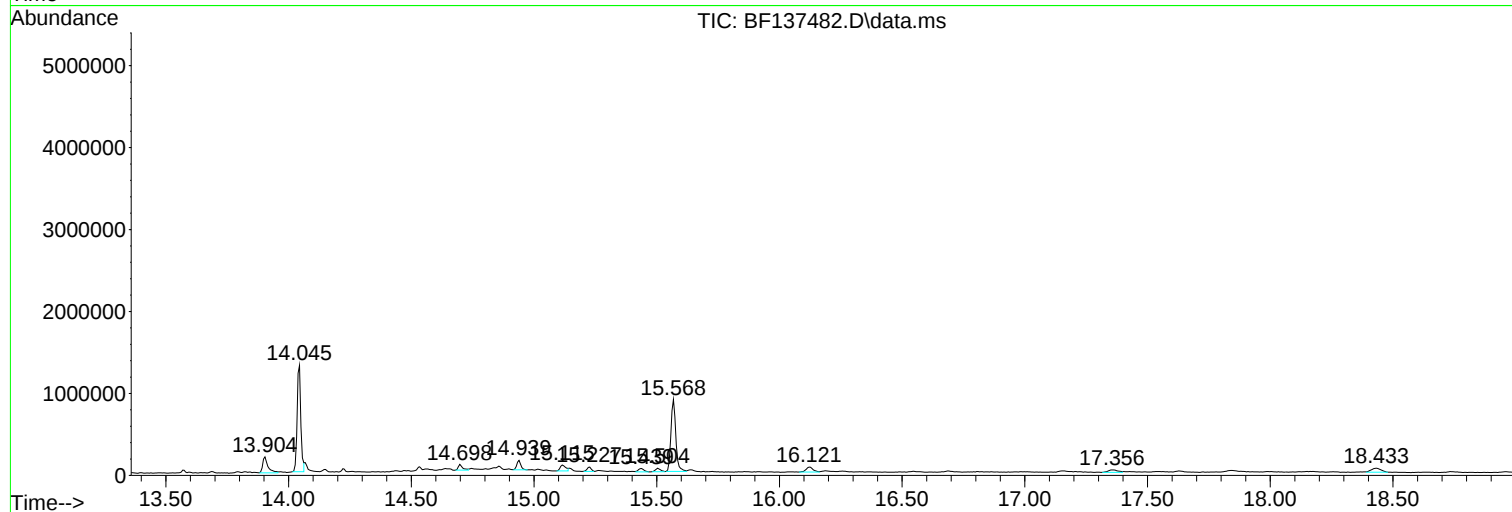
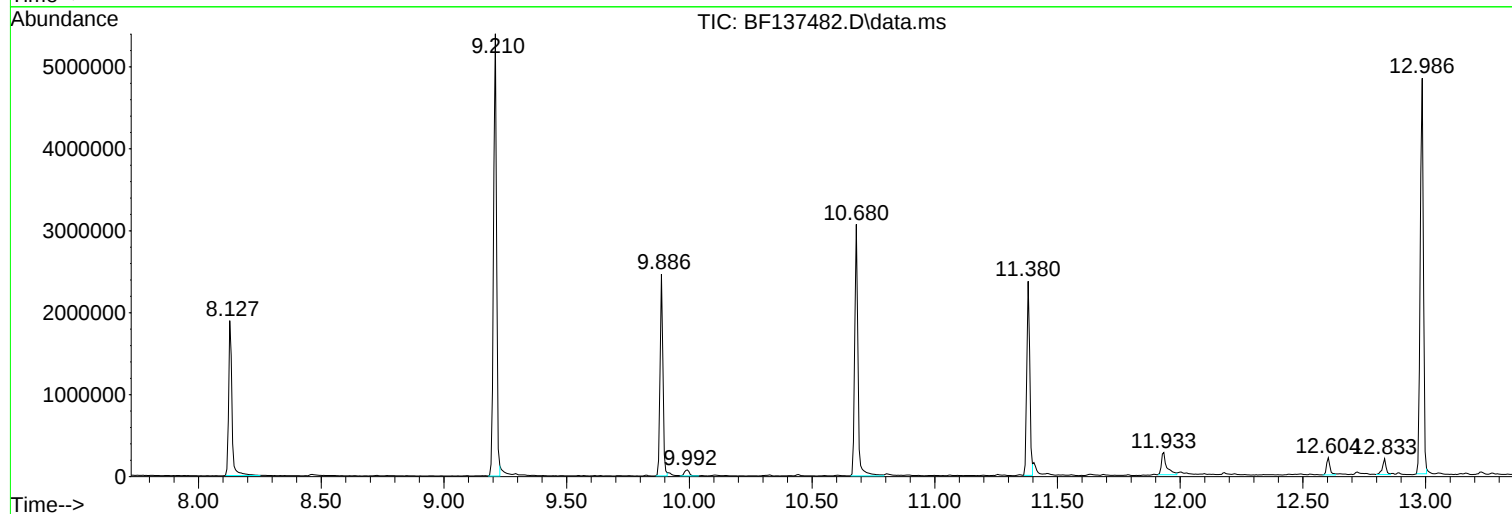
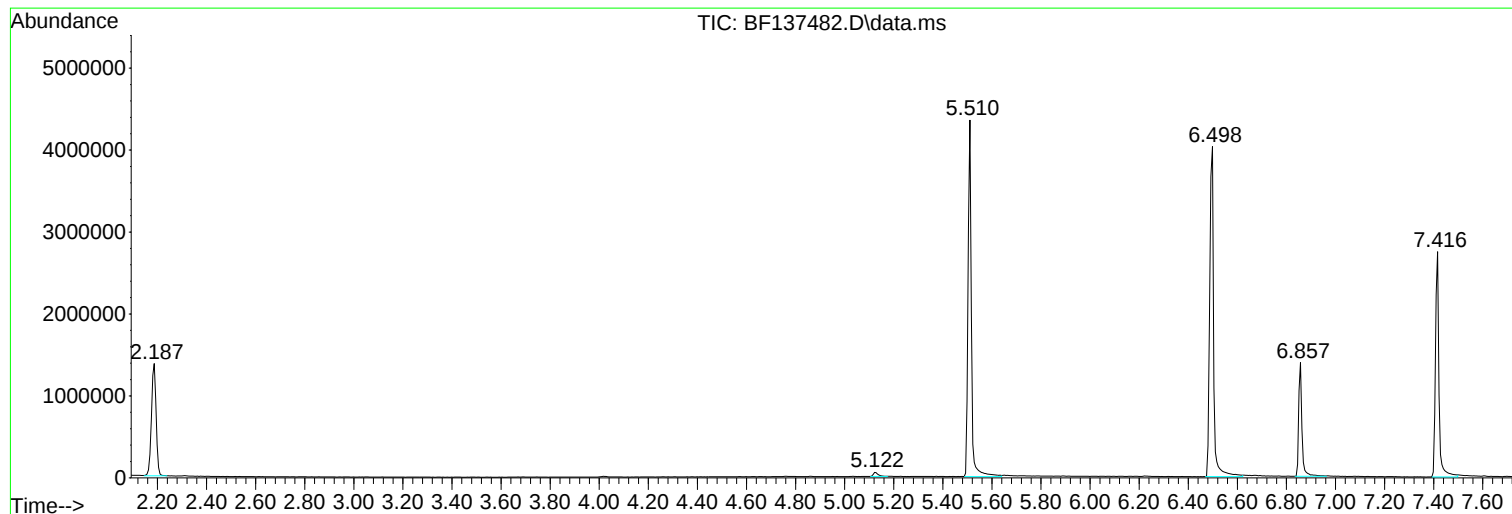
Sum of corrected areas: 36582357

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030424\
Data File : BF137482.D
Acq On : 04 Mar 2024 15:49
Operator : CG\JU
Sample : P1662-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-2520556

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.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\BF030424\
Data File : BF137482.D
Acq On : 04 Mar 2024 15:49
Operator : CG\JU
Sample : P1662-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-2520556

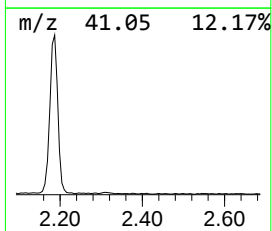
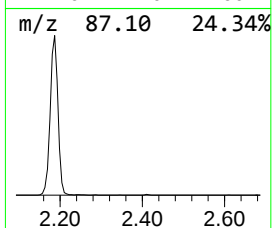
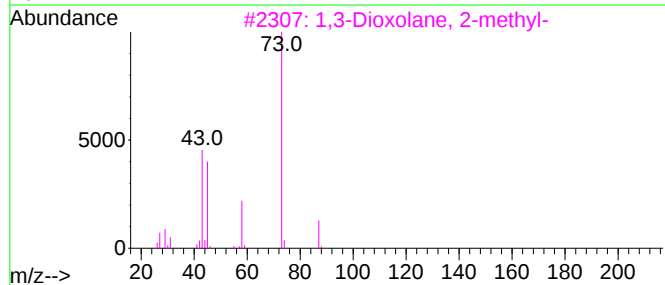
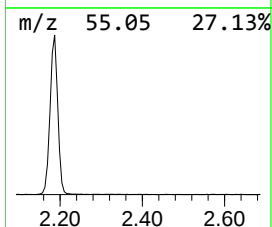
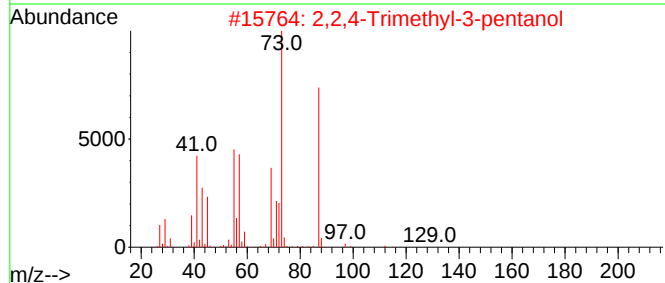
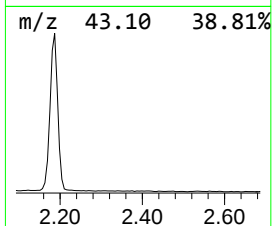
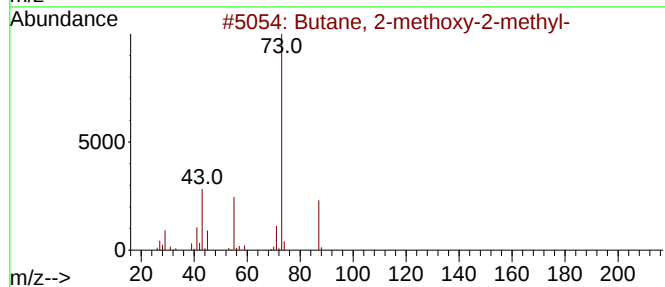
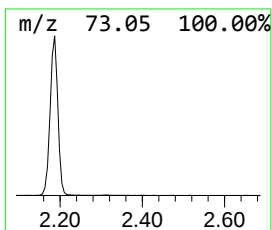
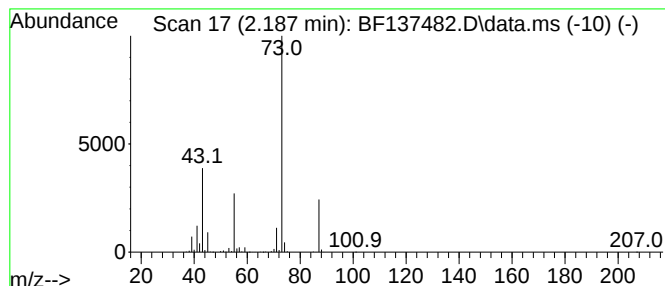
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	28.08 ng	1806450	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030424\
Data File : BF137482.D
Acq On : 04 Mar 2024 15:49
Operator : CG\JU
Sample : P1662-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-2520556

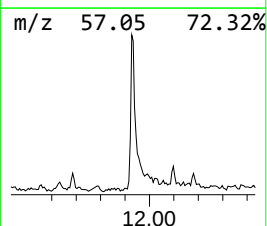
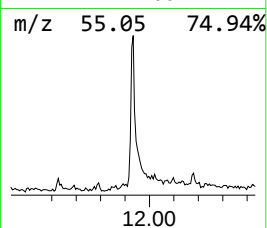
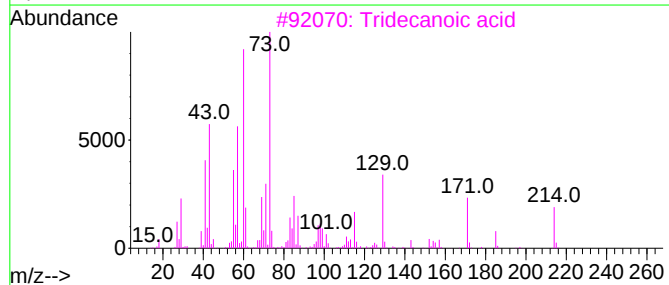
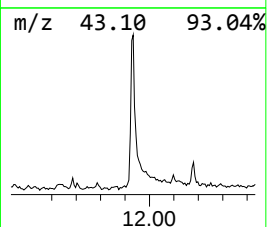
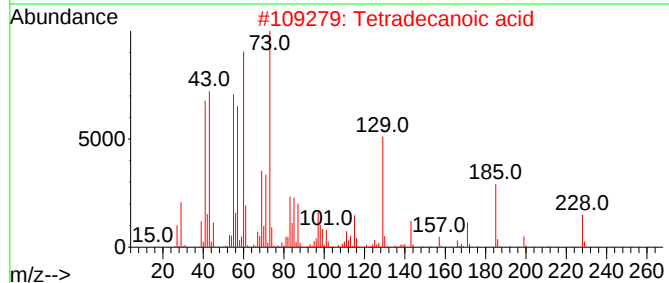
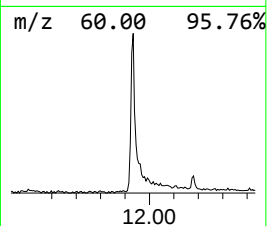
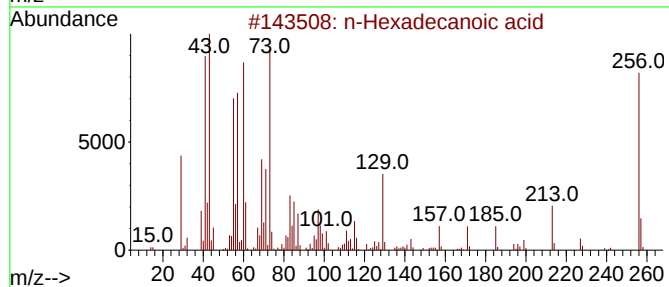
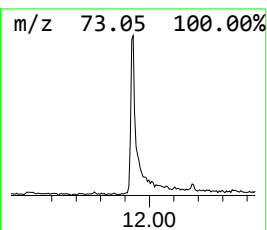
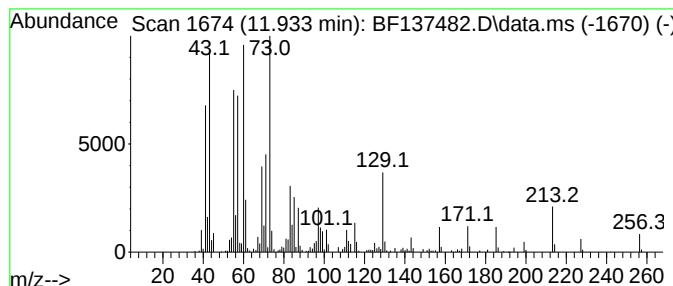
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	4.09 ng	406557	Phenanthrene-d10	11.380

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	95
3			Tridecanoic acid	214	C13H26O2	000638-53-9	81
4			Undecanoic acid	186	C11H22O2	000112-37-8	81
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030424\
Data File : BF137482.D
Acq On : 04 Mar 2024 15:49
Operator : CG\JU
Sample : P1662-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-2520556

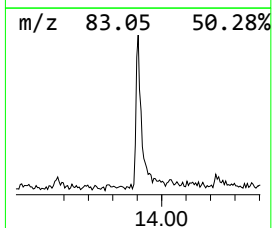
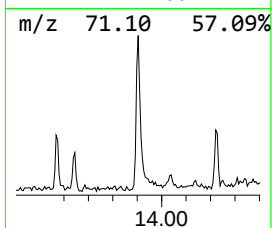
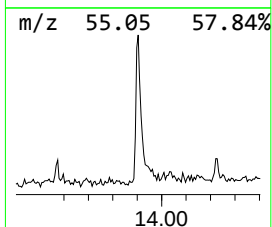
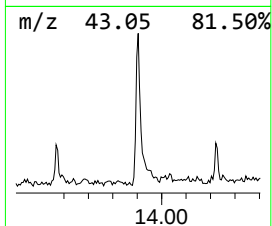
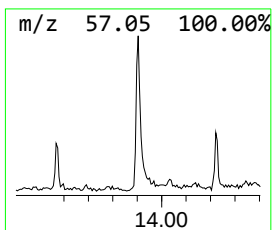
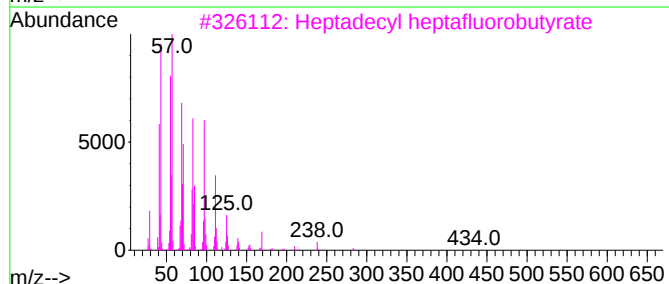
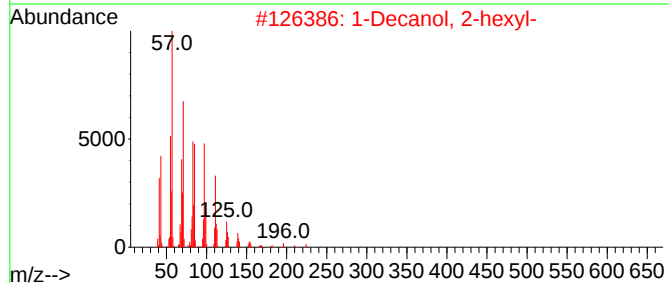
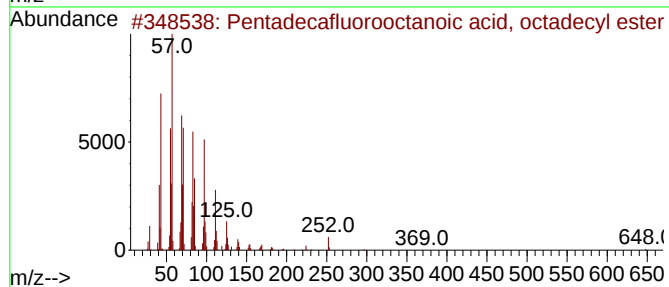
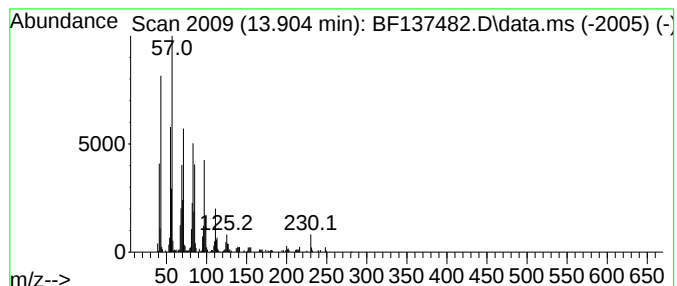
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	4.34 ng	295227	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	83
2			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	83
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	76
4			1-Hexacosanol	382	C26H54O	000506-52-5	76
5			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030424\
Data File : BF137482.D
Acq On : 04 Mar 2024 15:49
Operator : CG\JU
Sample : P1662-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-2520556

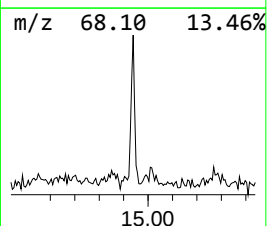
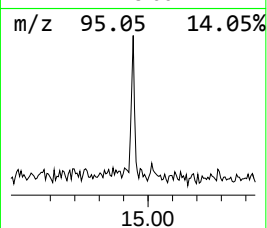
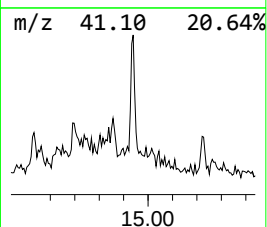
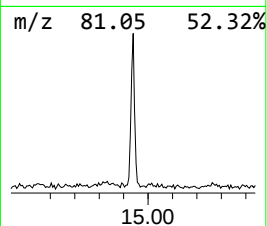
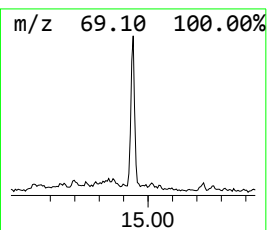
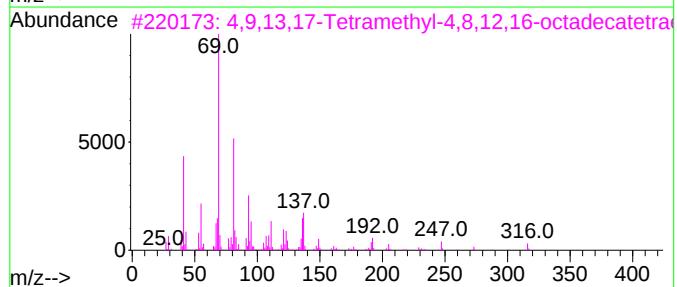
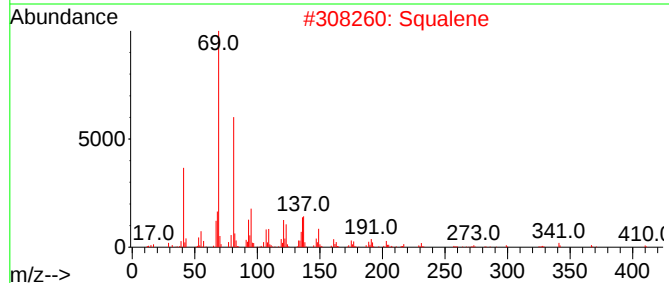
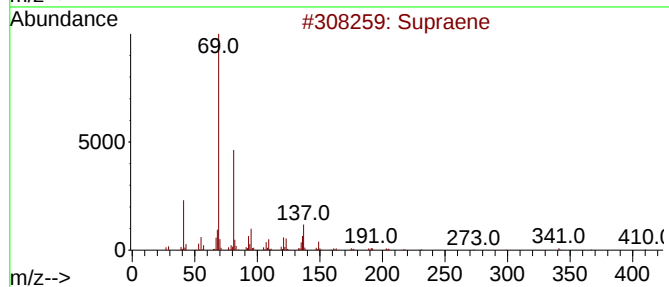
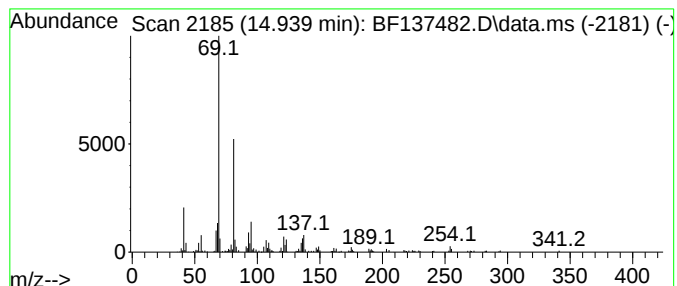
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.939	2.17 ng	129862	Perylene-d12	15.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	91
3			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
4			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	78
5			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030424\
Data File : BF137482.D
Acq On : 04 Mar 2024 15:49
Operator : CG\JU
Sample : P1662-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-2520556

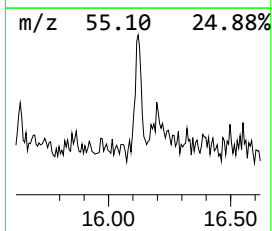
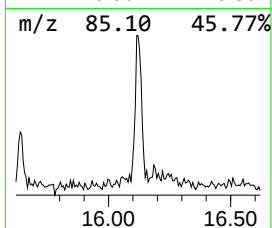
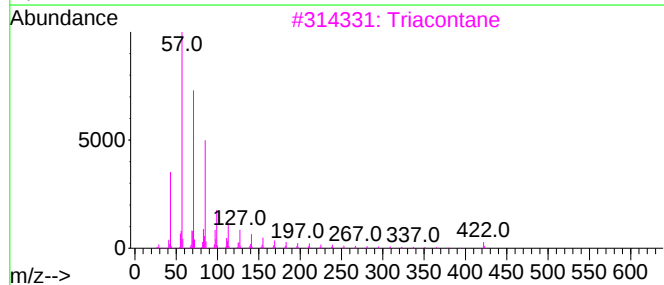
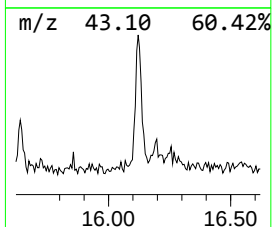
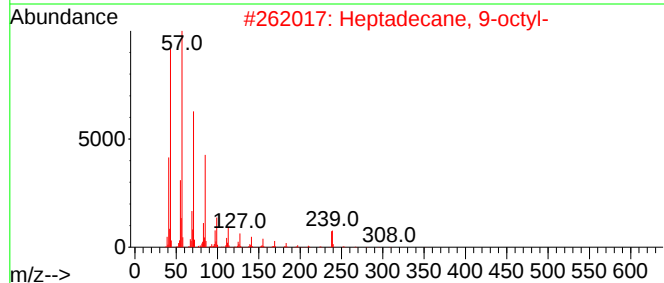
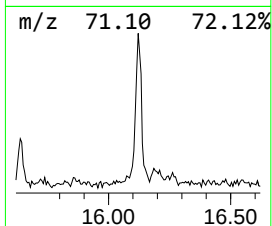
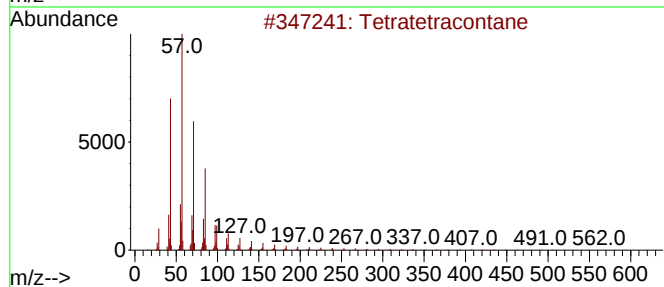
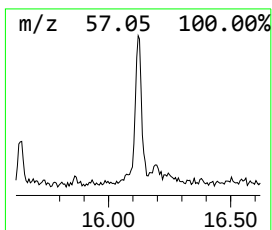
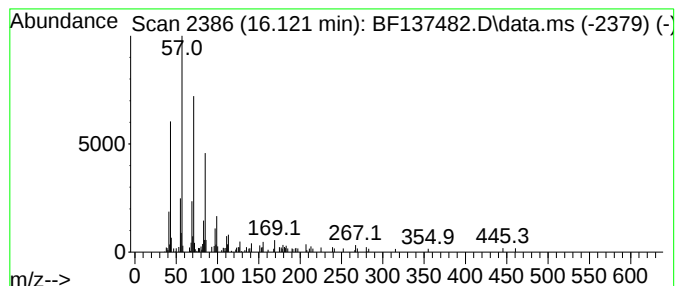
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetratetracontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.121	2.06 ng	123096	Perylene-d12	15.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	87
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
3			Triacontane	422	C30H62	000638-68-6	86
4			Tetratriacontane, 2-methyl-	493	C35H72	014167-65-8	86
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030424\
Data File : BF137482.D
Acq On : 04 Mar 2024 15:49
Operator : CG\JU
Sample : P1662-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-2520556

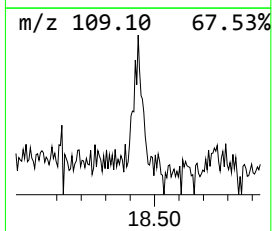
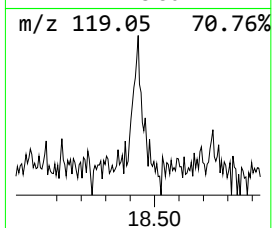
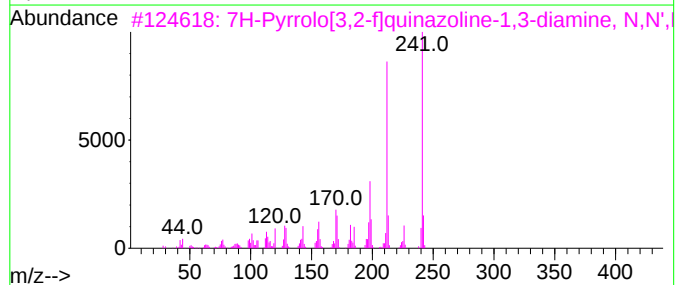
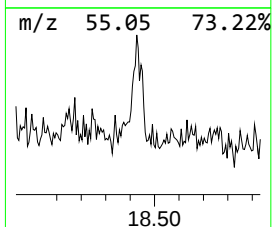
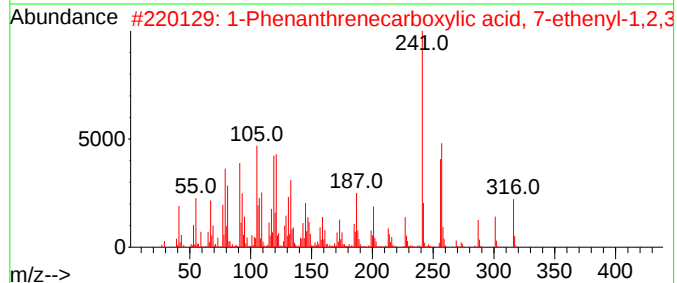
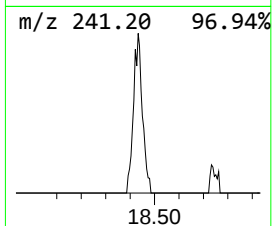
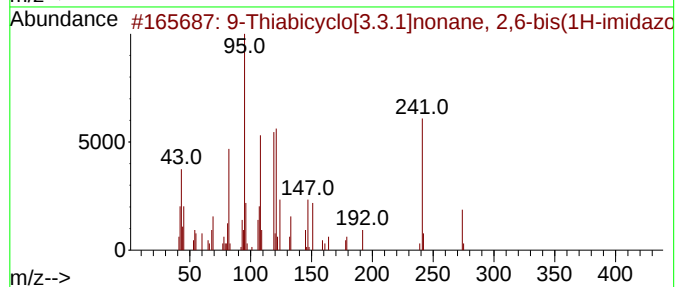
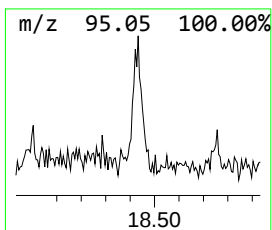
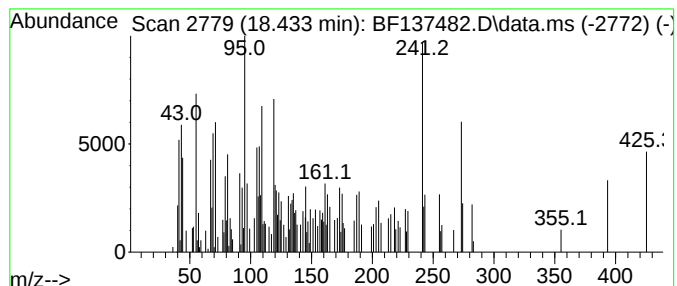
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown18.433 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.433	2.16 ng	128979	Perylene-d12	15.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Thiabicyclo[3.3.1]nonane, 2,6-...	274	C14H18N4S	1000141-52-1	14		
2	1-Phenanthrenecarboxylic acid, 7...	316	C21H32O2	001686-62-0	12		
3	7H-Pyrrolo[3,2-f]quinazoline-1,3...	241	C13H15N5	1000496-49-8	11		
4	2-Hydrazinyl-4-phenyl-1,3-benzot...	241	C13H11N3S	1000411-13-5	11		
5	propanedinitrile, 2-[5,5-dimethy...	241	C15H19N3	1000401-22-1	10		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030424\
Data File : BF137482.D
Acq On : 04 Mar 2024 15:49
Operator : CG\JU
Sample : P1662-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-2520556

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.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
Butane, 2-metho...	2.187	28.1	ng	1806450	1	6.857	1286550	20.0
n-Hexadecanoic ...	11.933	4.1	ng	406557	4	11.380	1985890	20.0
Pentadecafluoro...	13.904	4.3	ng	295227	5	14.045	1359510	20.0
Supraene	14.939	2.2	ng	129862	6	15.568	1196400	20.0
Tetratetracontane	16.121	2.1	ng	123096	6	15.568	1196400	20.0
unknown18.433	18.433	2.2	ng	128979	6	15.568	1196400	20.0