

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
 Data File : BF129415.D
 Acq On : 28 Jul 2022 18:38
 Operator : CG\JU
 Sample : N3895-18
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RVE-56

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-BF072522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129415.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.134	481	484	493	rVB	73016	92202	1.38%	0.152%
2	5.516	544	549	552	rBV	5580903	5461246	81.68%	9.013%
3	6.522	714	720	723	rBV	4993418	5635207	84.29%	9.300%
4	6.881	777	781	785	rBV	1598539	1268326	18.97%	2.093%
5	7.451	872	878	881	rBV	3602791	3776814	56.49%	6.233%
6	8.163	995	999	1003	rBV	2030316	1709262	25.57%	2.821%
7	9.245	1177	1183	1186	rBV	6581513	6685744	100.00%	11.034%
8	9.675	1252	1256	1267	rBV	420276	412216	6.17%	0.680%
9	9.922	1292	1298	1302	rBV	2287885	1898188	28.39%	3.133%
10	10.716	1428	1433	1436	rBV	4282626	4062162	60.76%	6.704%
11	11.416	1548	1552	1554	rBV	1834321	1699448	25.42%	2.805%
12	11.933	1637	1640	1652	rVB2	430260	458629	6.86%	0.757%
13	12.627	1755	1758	1763	rBV	127487	140615	2.10%	0.232%
14	12.857	1791	1797	1803	rBV	174273	193633	2.90%	0.320%
15	12.998	1817	1821	1825	rBV	5091141	5124774	76.65%	8.457%
16	13.216	1855	1858	1862	rBV	90552	93590	1.40%	0.154%
17	13.674	1933	1936	1946	rVB3	52509	84063	1.26%	0.139%
18	13.904	1969	1975	1987	rBV3	353357	868076	12.98%	1.433%
19	14.057	1997	2001	2004	rBV	1218079	1068963	15.99%	1.764%
20	14.510	2074	2078	2081	rBV	248967	237939	3.56%	0.393%
21	14.545	2081	2084	2086	rBV4	66031	90517	1.35%	0.149%
22	14.815	2127	2130	2135	rVB	94758	97966	1.47%	0.162%
23	14.898	2141	2144	2150	rVB	105096	107233	1.60%	0.177%
24	14.968	2152	2156	2161	rBV	564365	544159	8.14%	0.898%
25	15.104	2176	2179	2185	rBV	51158	83875	1.25%	0.138%
26	15.162	2185	2189	2193	rVB	545196	581972	8.70%	0.960%
27	15.221	2194	2199	2215	rBV3	282219	867159	12.97%	1.431%
28	15.551	2249	2255	2264	rVB	975418	1281465	19.17%	2.115%
29	15.762	2286	2291	2300	rBV	537986	792926	11.86%	1.309%
30	15.998	2325	2331	2340	rVB	890115	1398748	20.92%	2.308%
31	16.092	2341	2347	2350	rBV2	248188	594756	8.90%	0.982%
32	16.815	2465	2470	2476	rBV	320970	629076	9.41%	1.038%
33	17.121	2515	2522	2530	rVB	582308	1348715	20.17%	2.226%
34	17.227	2531	2540	2548	rBV	2590909	5708139	85.38%	9.420%
35	17.562	2591	2597	2609	rVB3	421004	1020019	15.26%	1.683%
36	17.680	2610	2617	2628	rBV7	187165	730669	10.93%	1.206%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129415.D
Acq On : 28 Jul 2022 18:38
Operator : CG\JU
Sample : N3895-18
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-56

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-BF072522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.786	2631	2635	2640	rVB3	147105	279774	4.18%	0.462%
38	18.074	2676	2684	2693	rVB7	410273	1082828	16.20%	1.787%
39	18.286	2712	2720	2731	rVB	380305	1063102	15.90%	1.754%
40	18.433	2738	2745	2754	rVB3	231890	622058	9.30%	1.027%
41	18.698	2783	2790	2805	rVB4	232209	698535	10.45%	1.153%

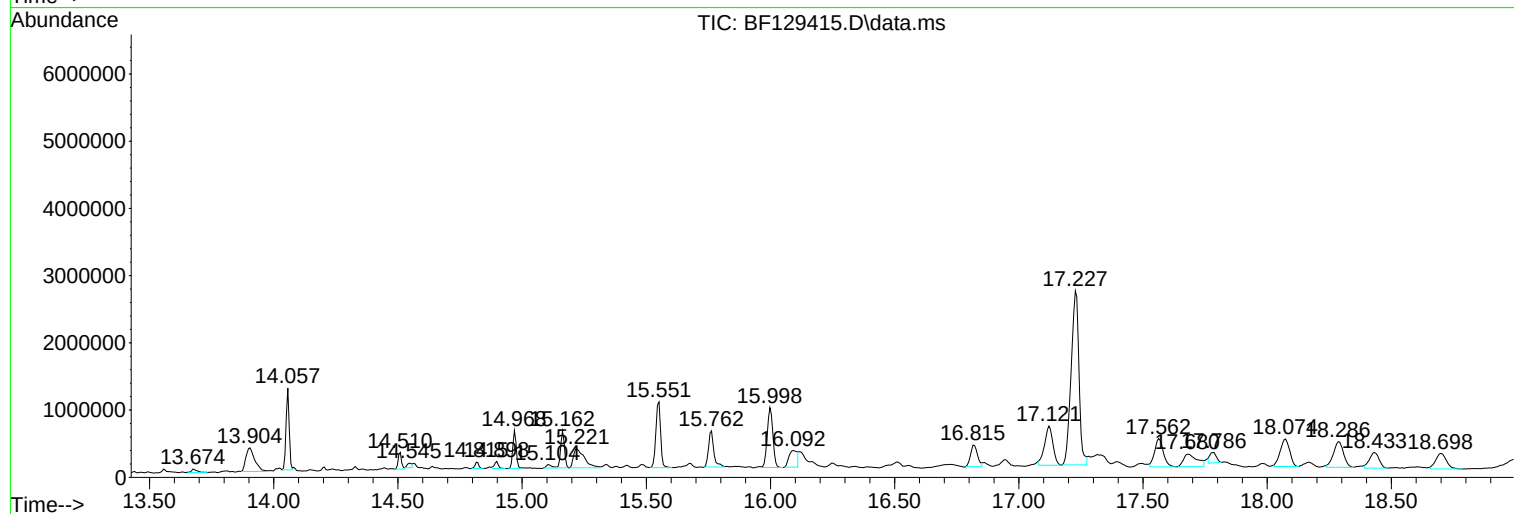
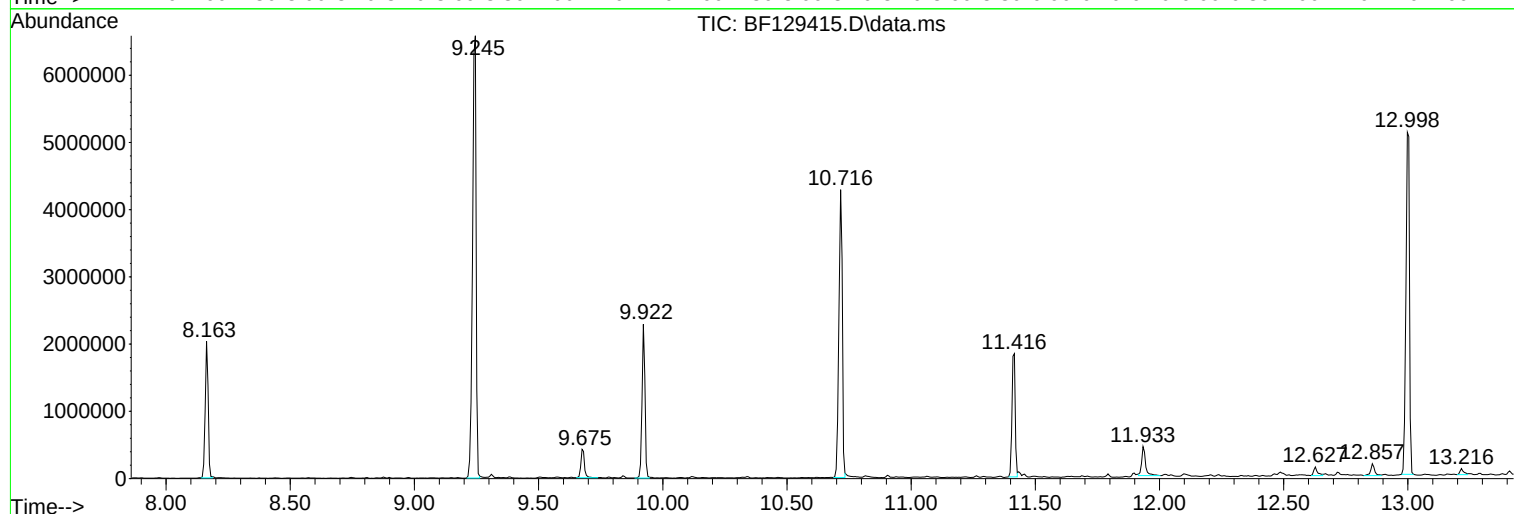
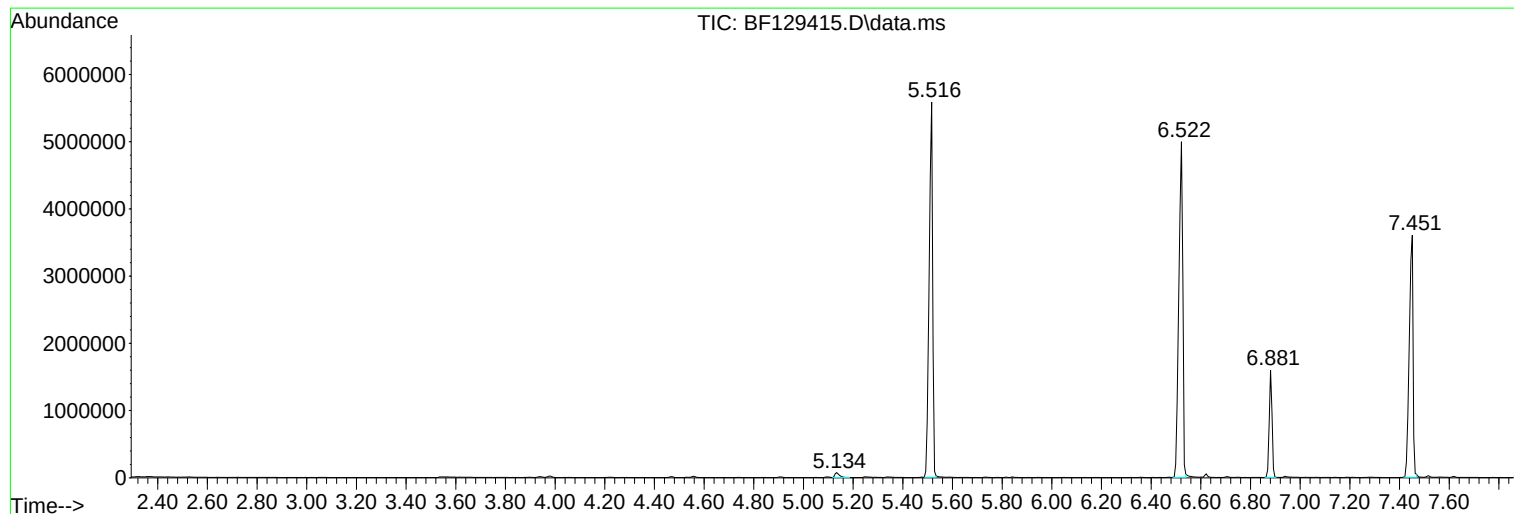
Sum of corrected areas: 60594788

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129415.D
Acq On : 28 Jul 2022 18:38
Operator : CG\JU
Sample : N3895-18
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-56

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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\BF072822\
Data File : BF129415.D
Acq On : 28 Jul 2022 18:38
Operator : CG\JU
Sample : N3895-18
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-56

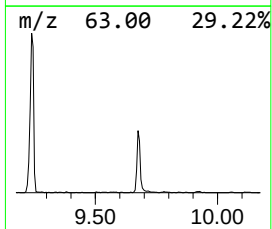
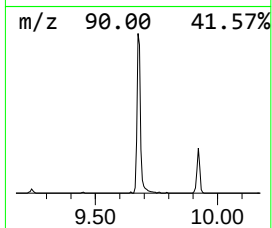
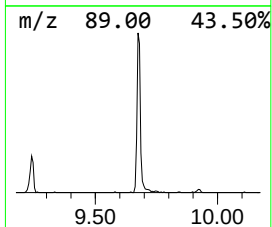
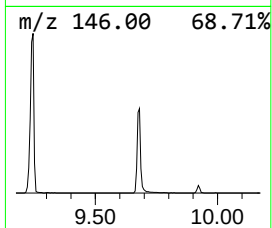
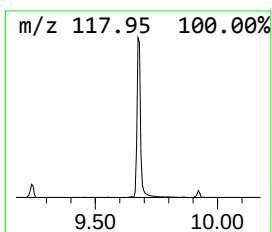
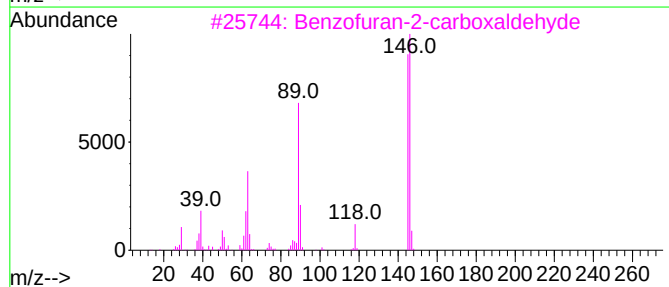
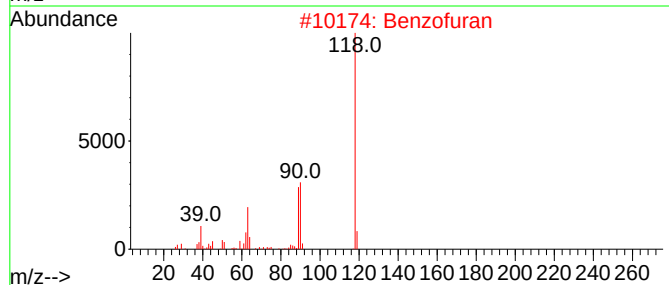
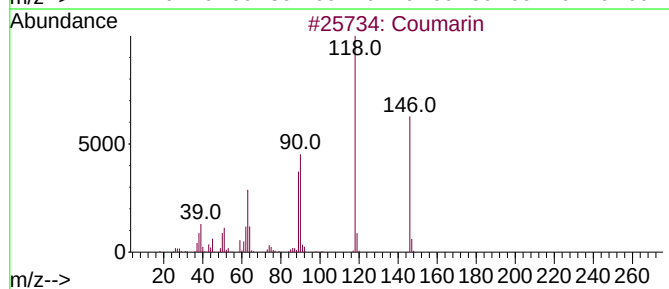
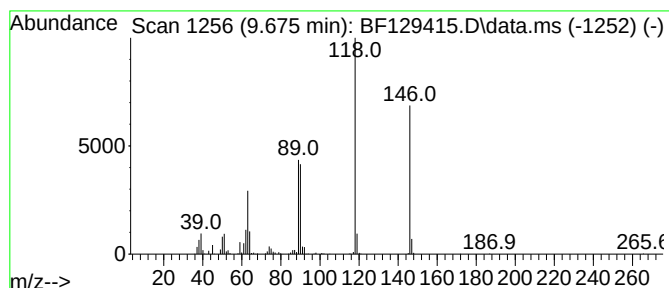
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Coumarin Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.675	4.34 ng	412216	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Coumarin	146	C9H6O2	000091-64-5	98
2			Benzofuran	118	C8H6O	000271-89-6	93
3			Benzofuran-2-carboxaldehyde	146	C9H6O2	004265-16-1	49
4			Phthalazin-1-one	146	C8H6N2O	000119-39-1	49
5			2H-Cyclopenta[d]pyridazine	118	C7H6N2	000270-64-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129415.D
Acq On : 28 Jul 2022 18:38
Operator : CG\JU
Sample : N3895-18
Misc :
ALS Vial : 7 Sample Multiplier: 1

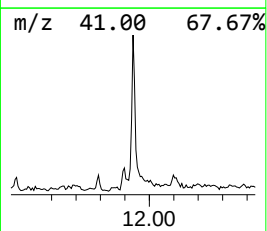
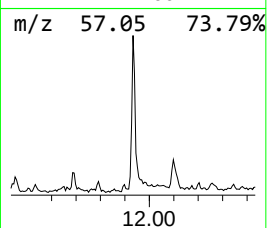
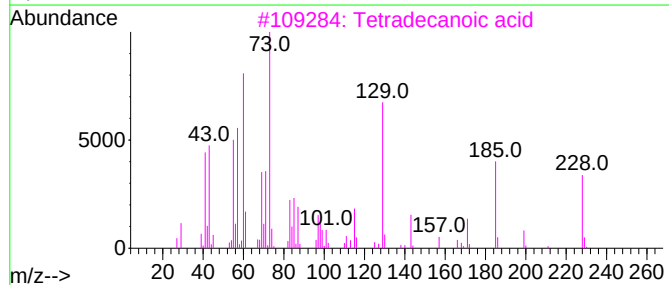
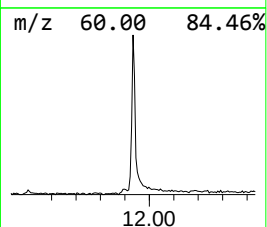
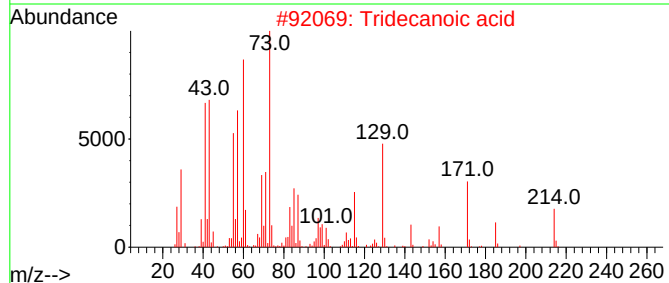
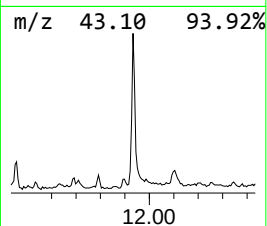
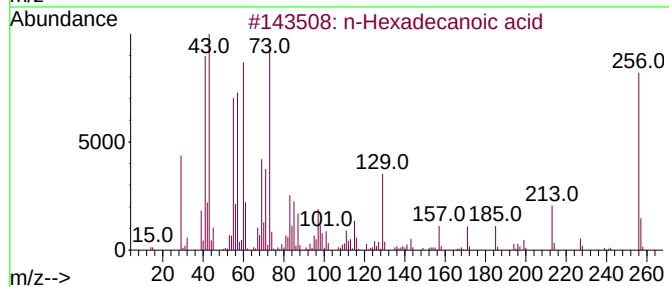
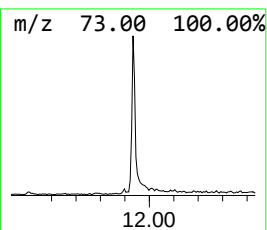
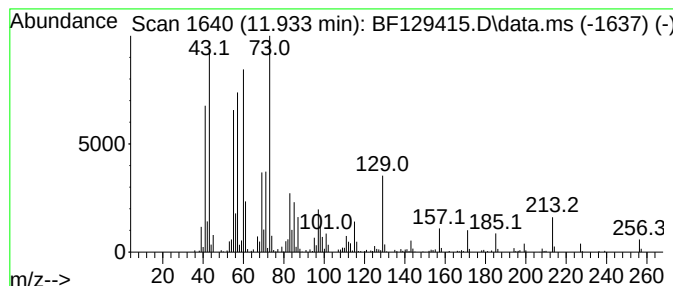
Instrument :
BNA_F
ClientSampleId :
RVE-56

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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 17

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.933	5.40 ng	458629	Phenanthrene-d10	11.416	
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	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129415.D
Acq On : 28 Jul 2022 18:38
Operator : CG\JU
Sample : N3895-18
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-56

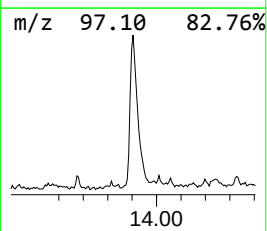
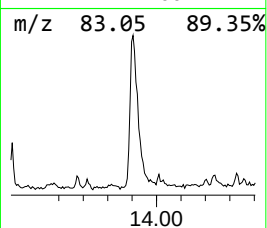
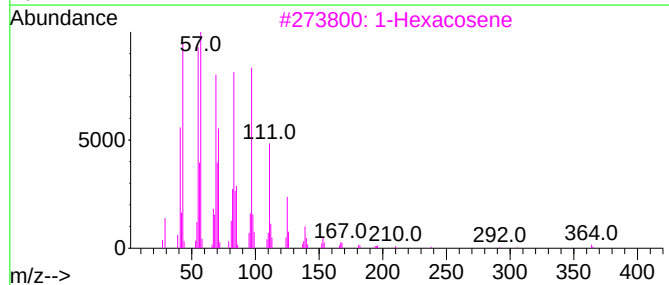
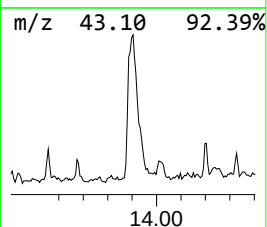
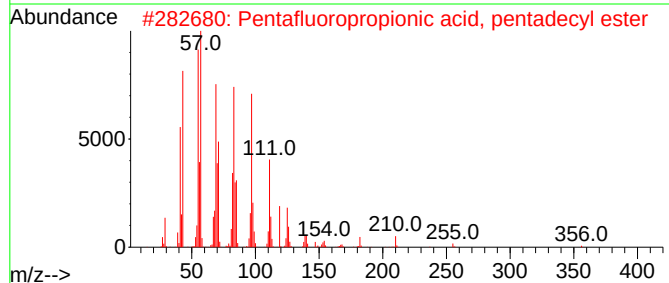
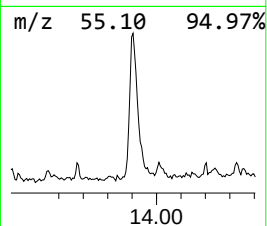
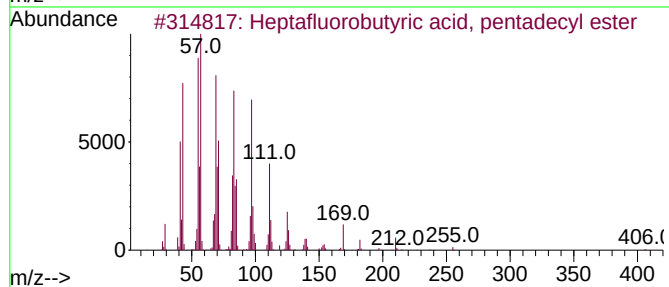
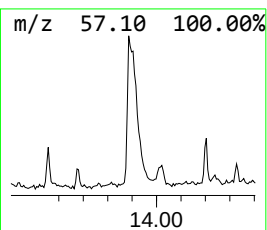
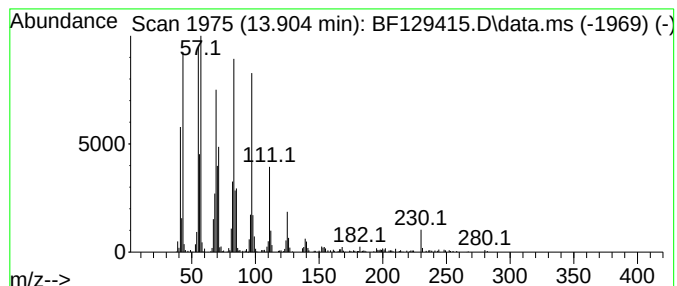
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Heptafluorobutyric acid, pe... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	16.24 ng	868076	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3			1-Hexacosene	364	C26H52	018835-33-1	94
4			1-Heneicosanol	312	C21H44O	015594-90-8	94
5			E-14-Hexadecenal	238	C16H30O	330207-53-9	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129415.D
Acq On : 28 Jul 2022 18:38
Operator : CG\JU
Sample : N3895-18
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-56

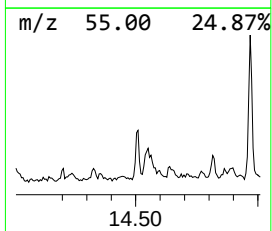
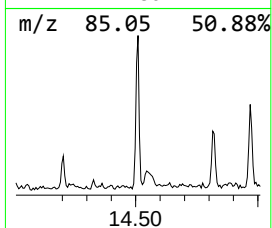
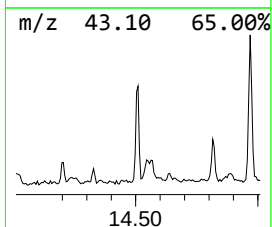
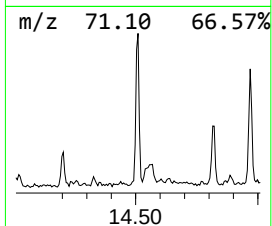
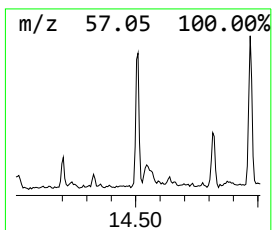
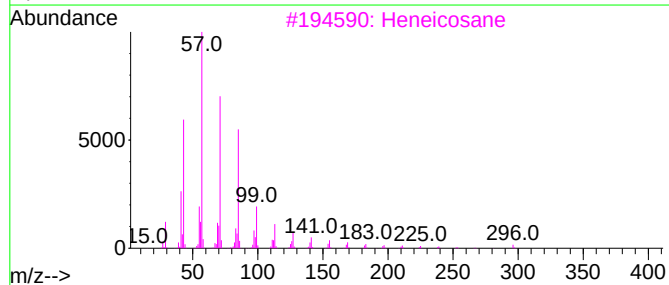
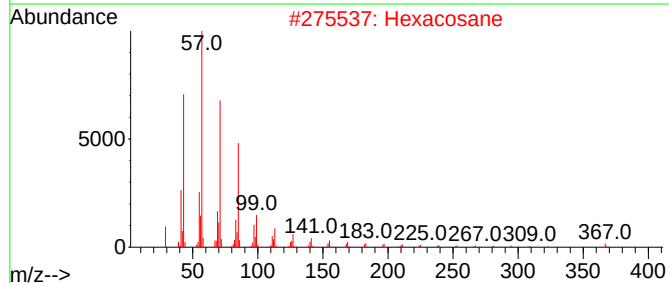
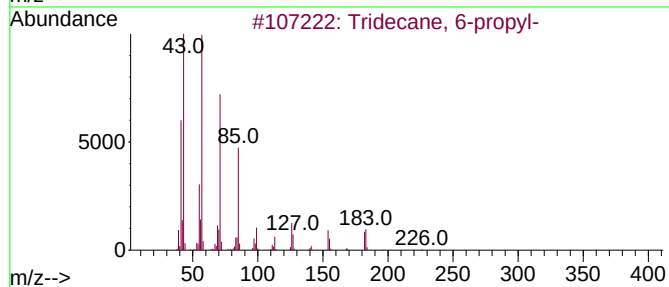
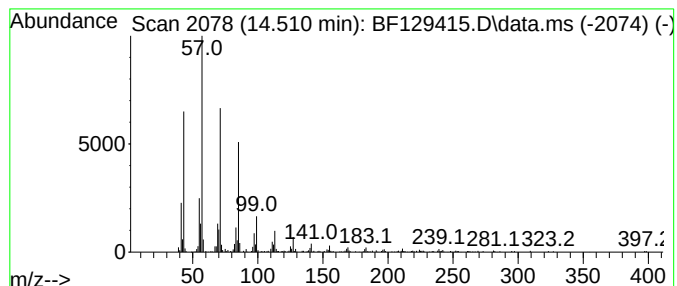
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tridecane, 6-propyl- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.510	4.45 ng	237939	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 6-propyl-	226	C16H34	055045-10-8	93
2			Hexacosane	366	C26H54	000630-01-3	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	91
5			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129415.D
Acq On : 28 Jul 2022 18:38
Operator : CG\JU
Sample : N3895-18
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-56

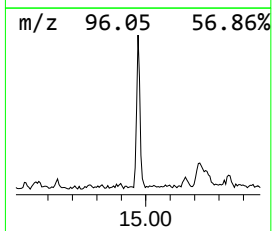
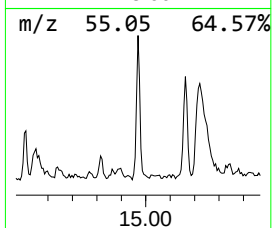
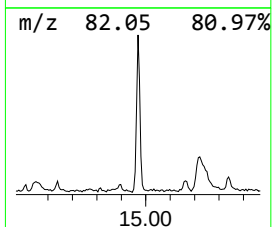
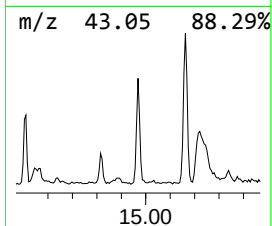
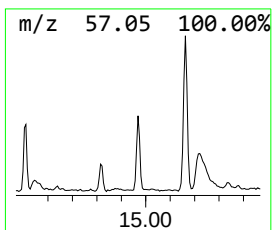
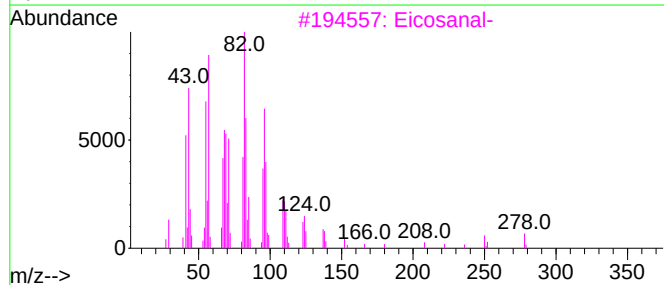
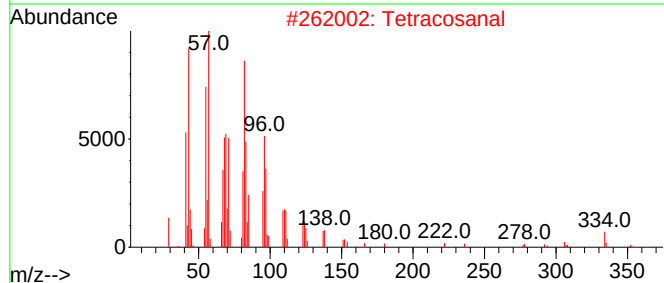
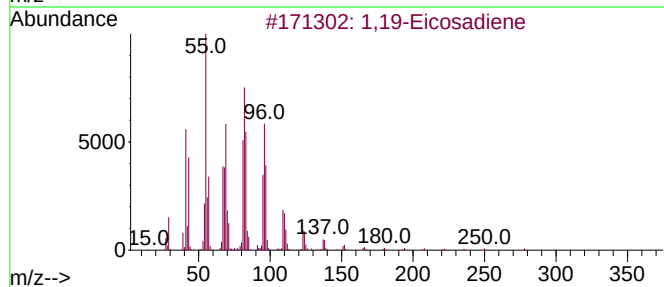
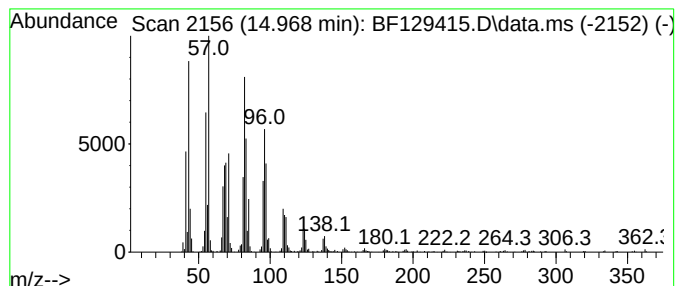
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1,19-Eicosadiene Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.968	8.49 ng	544159	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,19-Eicosadiene	278	C20H38	014811-95-1	95
2			Tetracosanal	352	C24H48O	057866-08-7	94
3			Eicosanal-	296	C20H40O	002400-66-0	94
4			Octadecanal	268	C18H36O	000638-66-4	91
5			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129415.D
Acq On : 28 Jul 2022 18:38
Operator : CG\JU
Sample : N3895-18
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-56

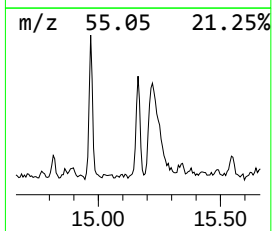
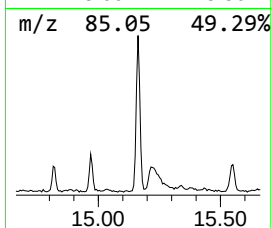
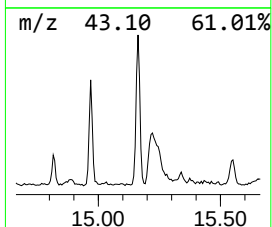
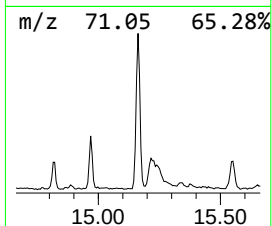
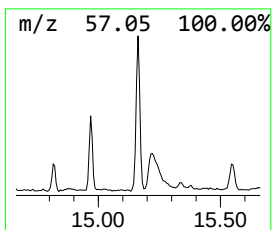
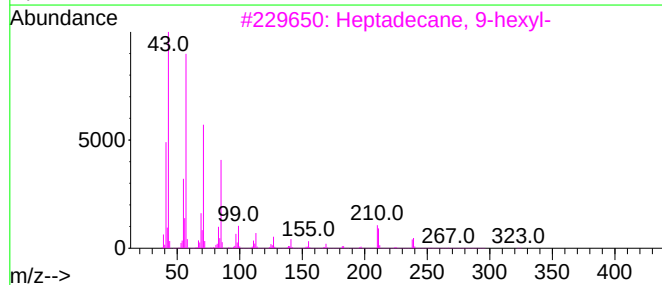
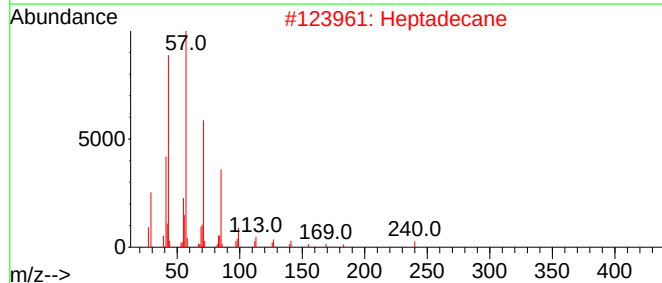
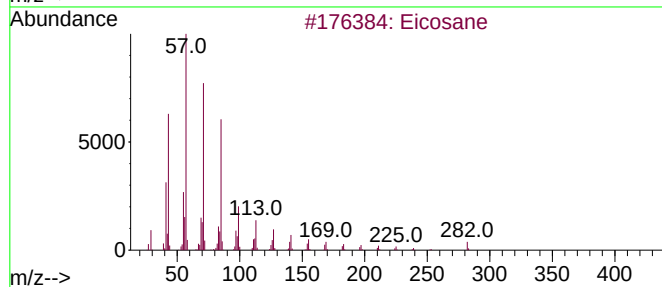
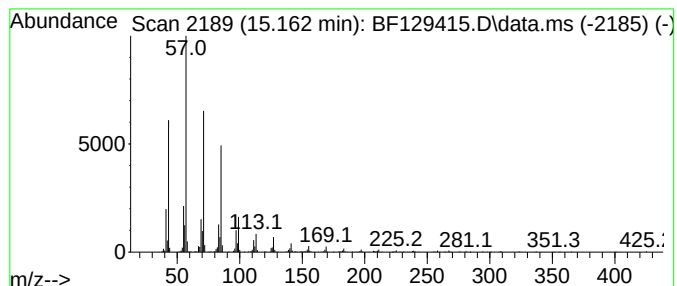
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Eicosane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.163	9.08 ng	581972	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	95
2			Heptadecane	240	C17H36	000629-78-7	94
3			Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	94
4			Heneicosane	296	C21H44	000629-94-7	91
5			Hexacosane	366	C26H54	000630-01-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129415.D
Acq On : 28 Jul 2022 18:38
Operator : CG\JU
Sample : N3895-18
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-56

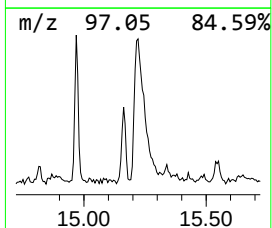
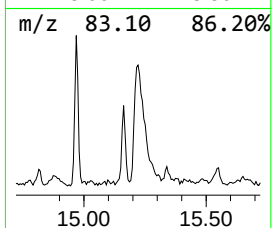
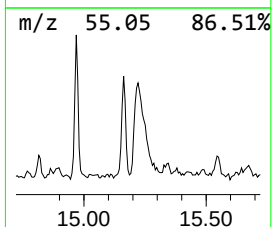
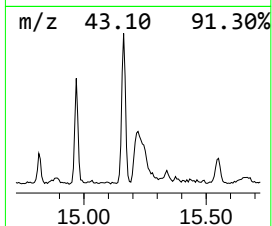
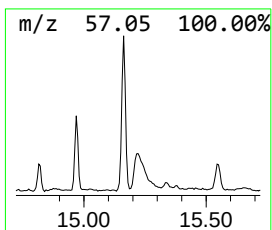
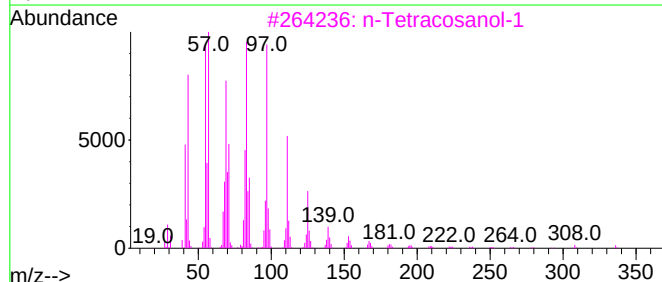
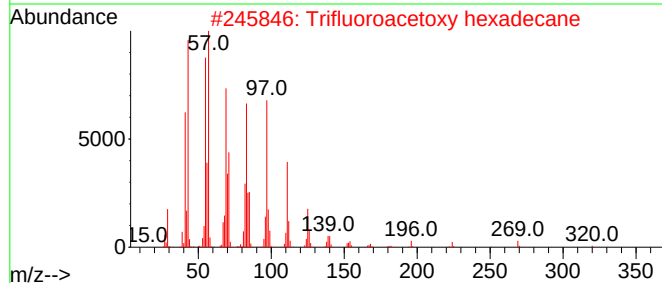
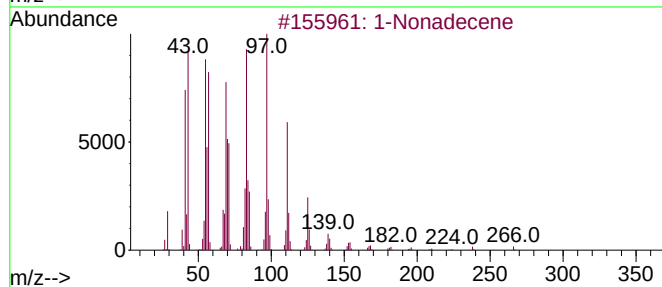
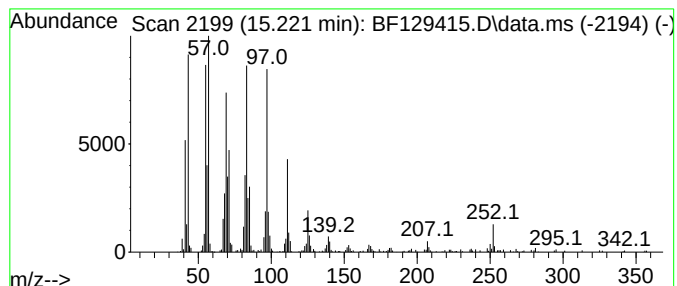
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Nonadecene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.221	13.53 ng	867159	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene			266	C19H38	018435-45-5	95
2	Trifluoroacetoxy hexadecane			338	C18H33F3O2	006222-03-3	94
3	n-Tetracosanol-1			354	C24H50O	000506-51-4	94
4	Trifluoroacetic acid, pentadecyl...			324	C17H31F3O2	959010-23-2	94
5	Behenic alcohol			326	C22H46O	000661-19-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129415.D
Acq On : 28 Jul 2022 18:38
Operator : CG\JU
Sample : N3895-18
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-56

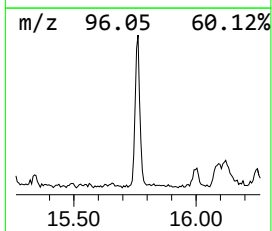
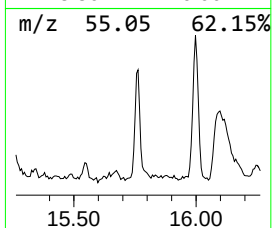
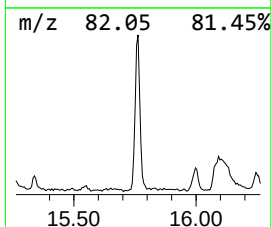
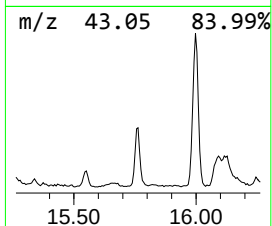
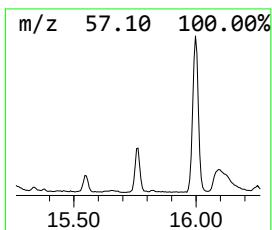
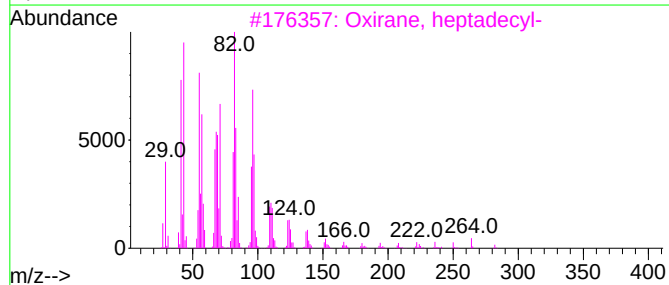
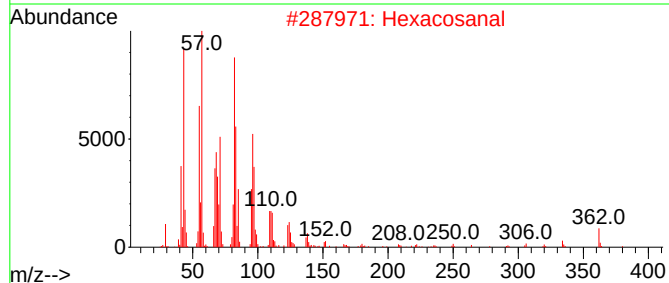
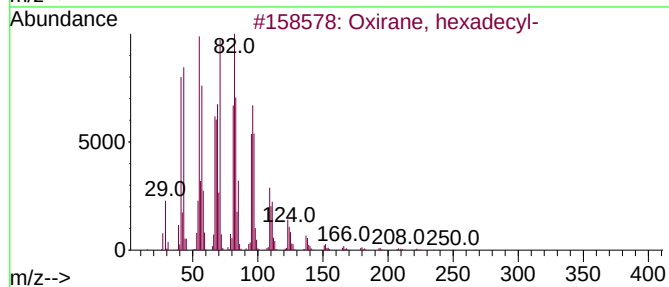
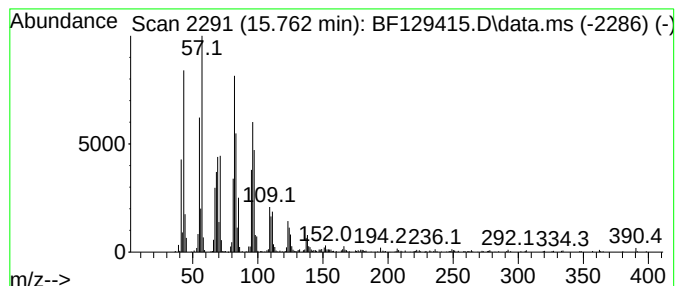
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Oxirane, hexadecyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.762	12.38 ng	792926	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
2			Hexacosanal	380	C26H52O	026627-85-0	91
3			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
4			Octadecanal	268	C18H36O	000638-66-4	90
5			1,19-Eicosadiene	278	C20H38	014811-95-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129415.D
Acq On : 28 Jul 2022 18:38
Operator : CG\JU
Sample : N3895-18
Misc :
ALS Vial : 7 Sample Multiplier: 1

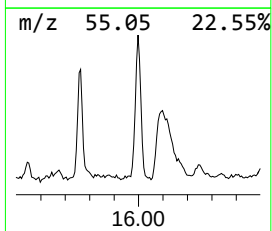
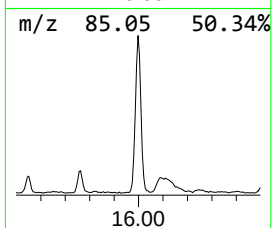
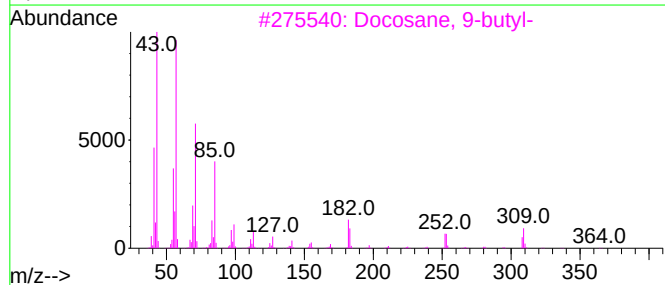
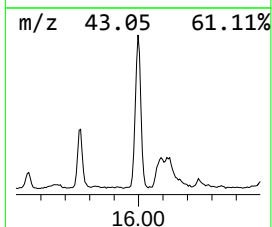
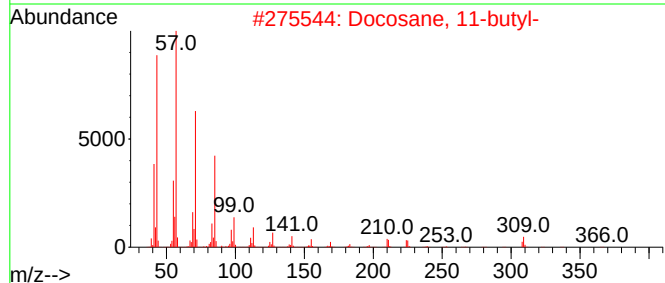
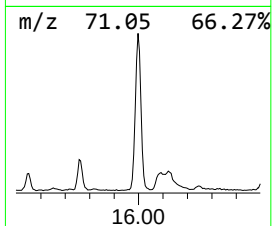
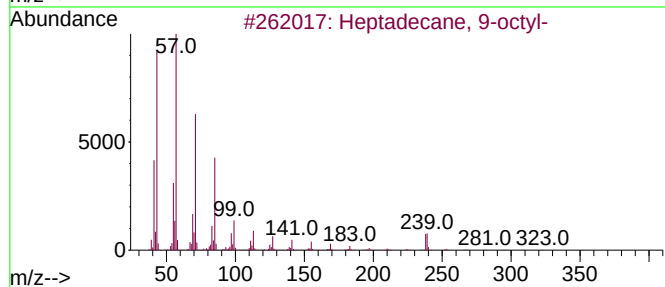
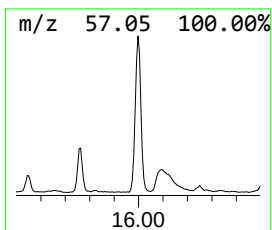
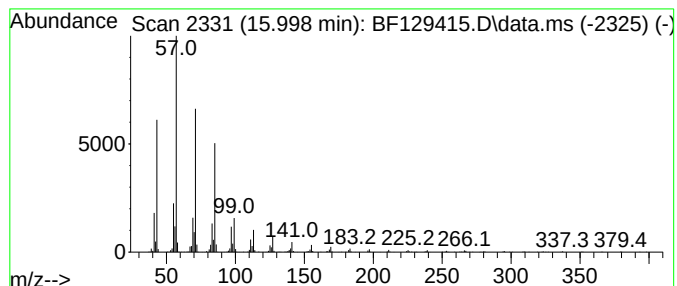
Instrument :
BNA_F
ClientSampleId :
RVE-56

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecane, 9-octyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.998	21.83 ng	1398750	Perylene-d12	15.551	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	95
2	Docosane, 11-butyl-	366	C26H54	013475-76-8	95
3	Docosane, 9-butyl-	366	C26H54	055282-14-9	94
4	Octacosane	394	C28H58	000630-02-4	91
5	Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129415.D
Acq On : 28 Jul 2022 18:38
Operator : CG\JU
Sample : N3895-18
Misc :
ALS Vial : 7 Sample Multiplier: 1

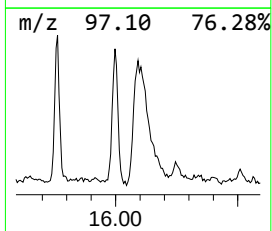
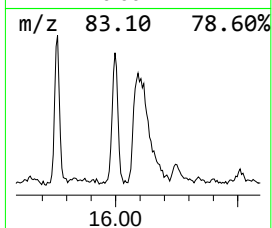
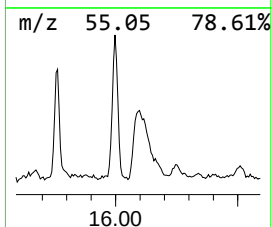
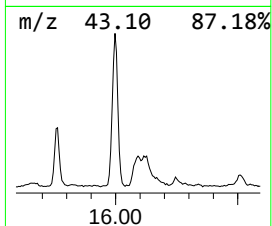
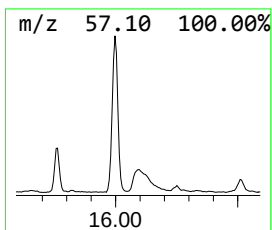
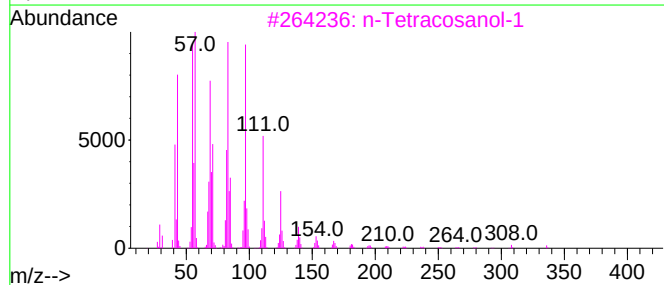
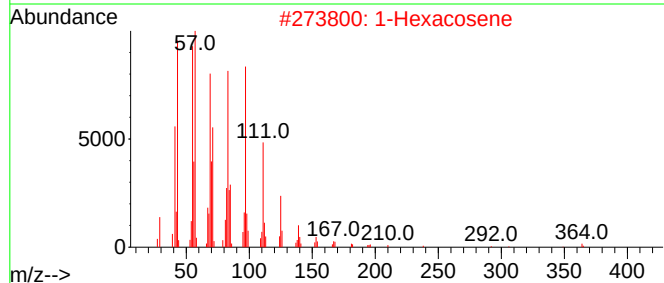
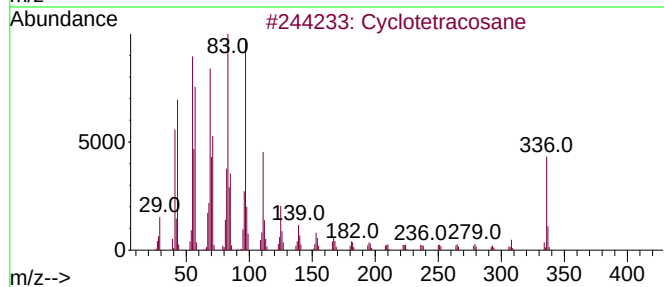
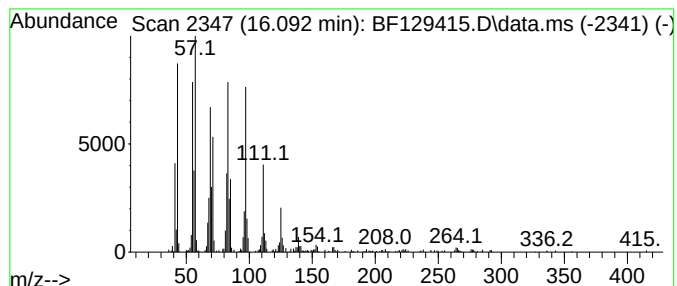
Instrument :
BNA_F
ClientSampleId :
RVE-56

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cyclotetracosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.092	9.28 ng	594756	Perylene-d12	15.551	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	97
2	1-Hexacosene	364	C26H52	018835-33-1	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5	Behenic alcohol	326	C22H46O	000661-19-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129415.D
Acq On : 28 Jul 2022 18:38
Operator : CG\JU
Sample : N3895-18
Misc :
ALS Vial : 7 Sample Multiplier: 1

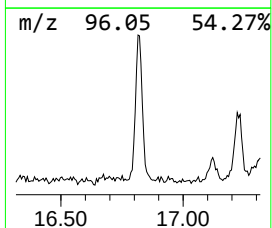
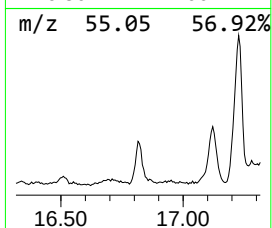
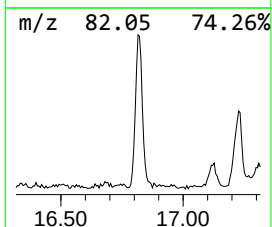
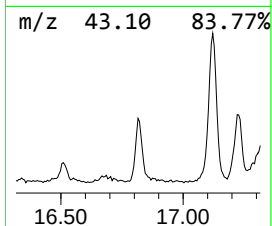
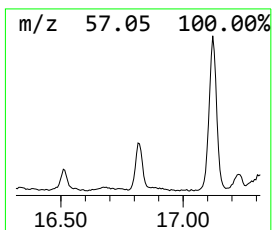
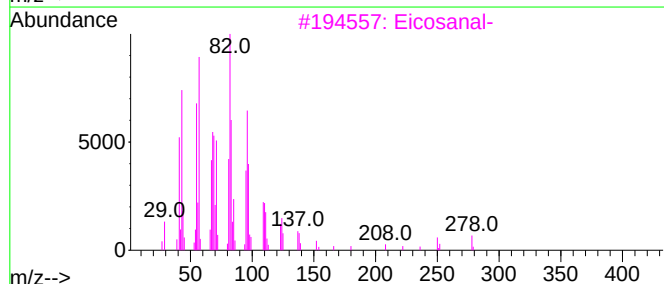
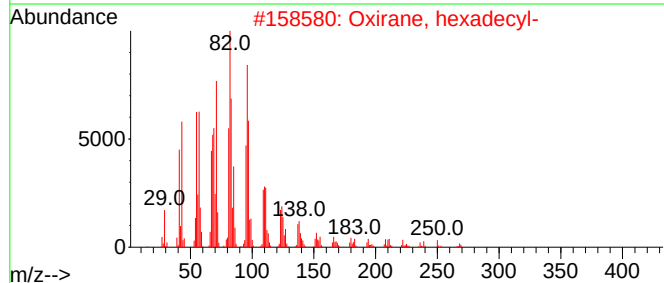
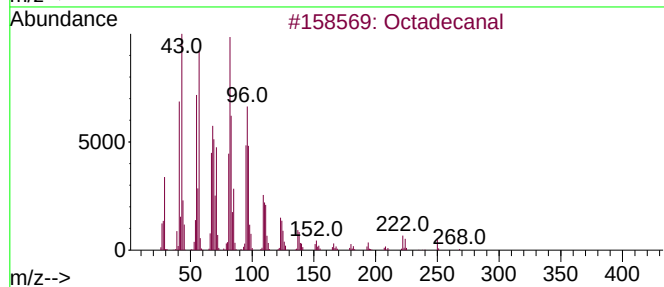
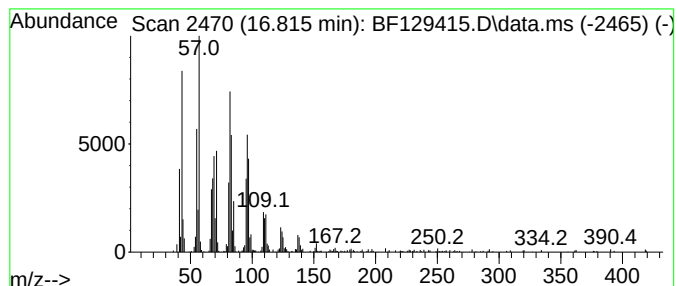
Instrument :
BNA_F
ClientSampleId :
RVE-56

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octadecanal Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.815	9.82 ng	629076	Perylene-d12	15.551	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	94
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3	Eicosanal-	296	C20H40O	002400-66-0	90
4	(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	90
5	Octacosanal	408	C28H56O	022725-64-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129415.D
Acq On : 28 Jul 2022 18:38
Operator : CG\JU
Sample : N3895-18
Misc :
ALS Vial : 7 Sample Multiplier: 1

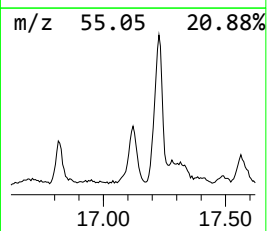
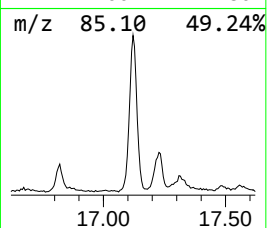
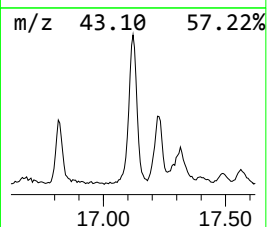
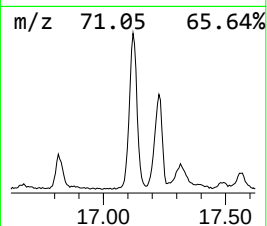
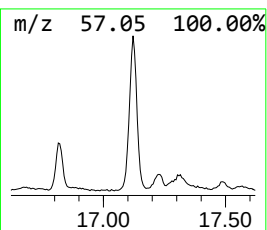
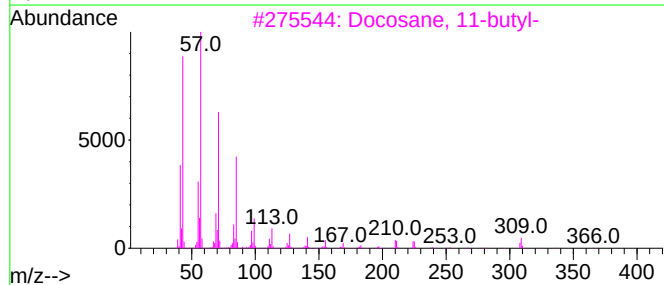
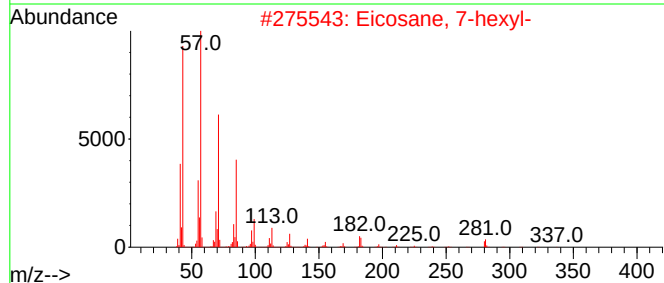
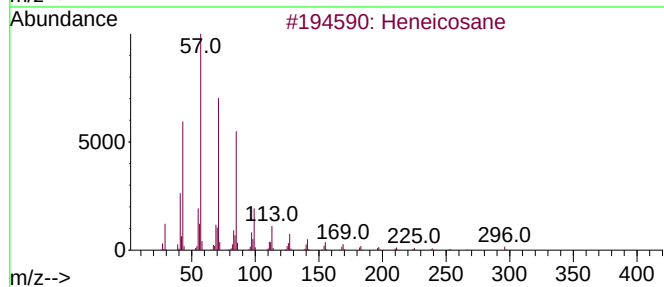
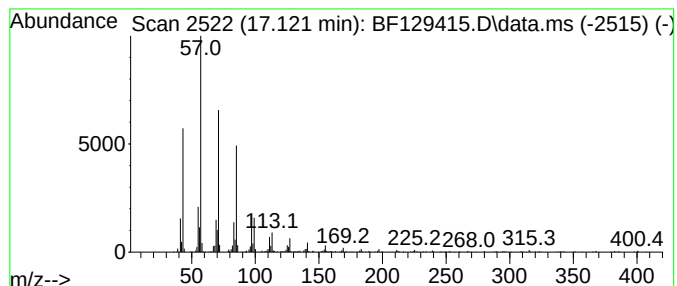
Instrument :
BNA_F
ClientSampleId :
RVE-56

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.121	21.05 ng	1348720	Perylene-d12	15.551	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129415.D
Acq On : 28 Jul 2022 18:38
Operator : CG\JU
Sample : N3895-18
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-56

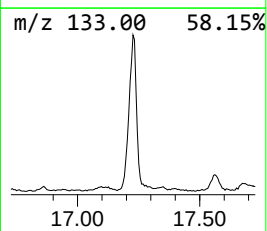
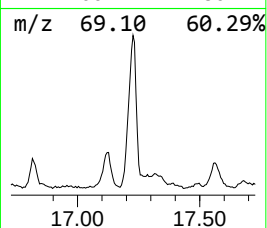
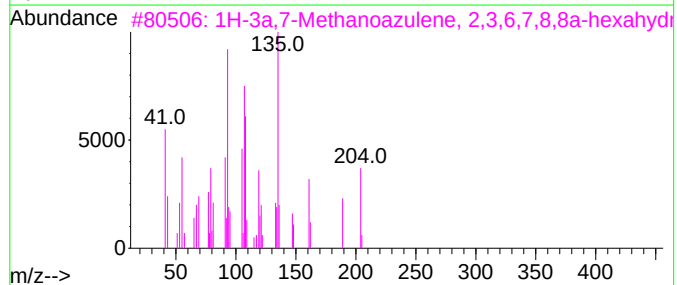
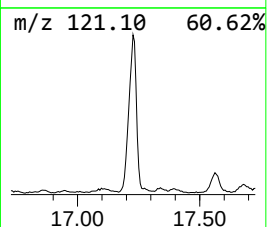
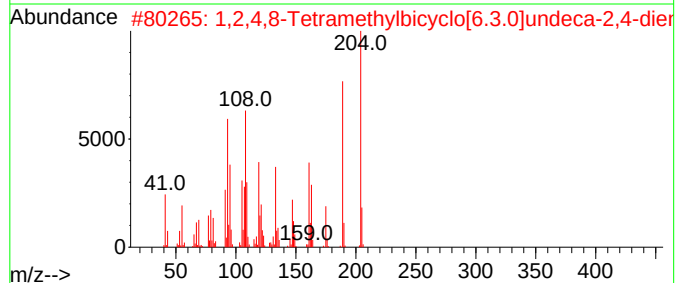
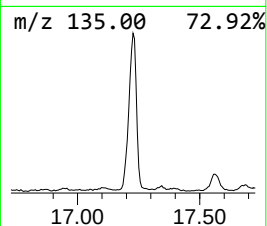
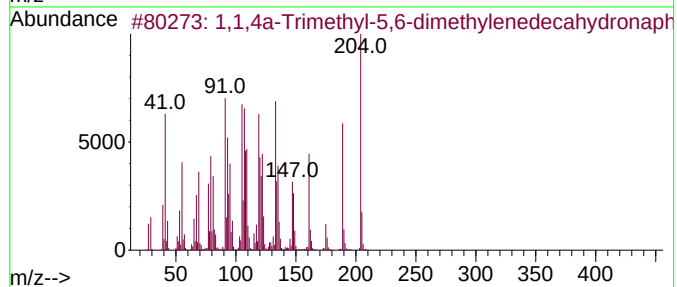
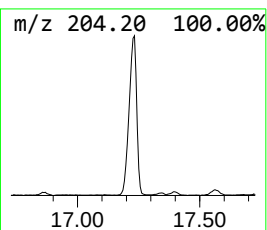
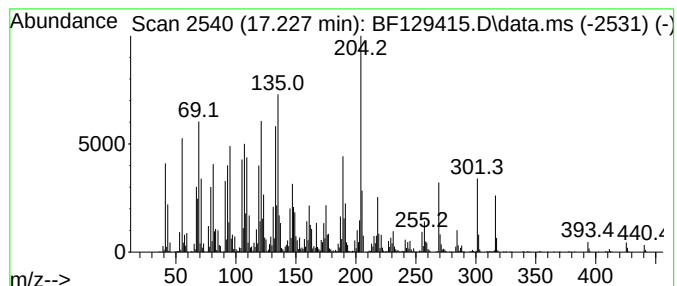
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1,1,4a-Trimethyl-5,6-dimeth... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.227	89.09 ng	5708140	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	81		
2	1,2,4,8-Tetramethylbicyclo[6.3.0]...	204	C15H24	137235-51-9	53		
3	1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	49		
4	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1010140-07-7	49		
5	Farnesyl bromide	284	C15H25Br	006874-67-5	47		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129415.D
Acq On : 28 Jul 2022 18:38
Operator : CG\JU
Sample : N3895-18
Misc :
ALS Vial : 7 Sample Multiplier: 1

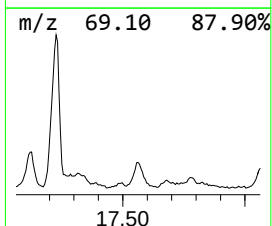
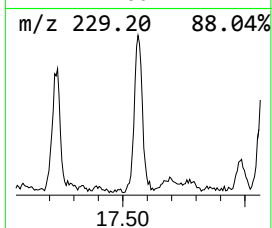
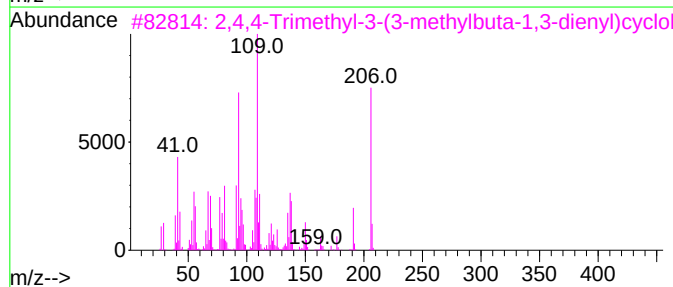
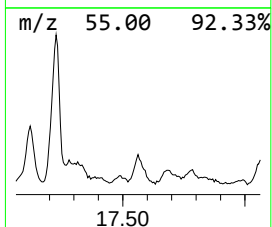
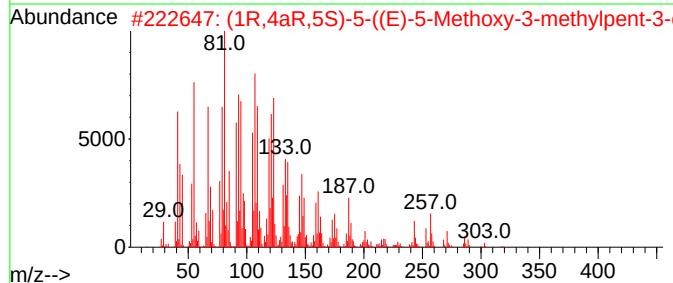
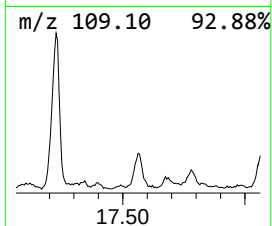
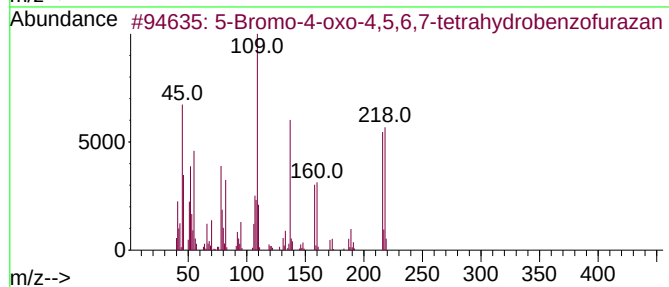
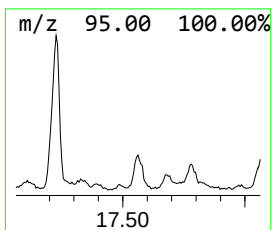
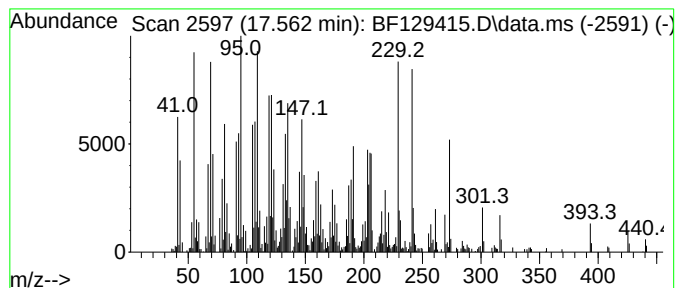
Instrument :
BNA_F
ClientSampleId :
RVE-56

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 5-Bromo-4-oxo-4,5,6,7-tetra... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.562	15.92 ng	1020020	Perylene-d12	15.551
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216 C6H5BrN2O2	300574-36-1 59
2		(1R,4aR,5S)-5-((E)-5-Methoxy-3-m...	318 C21H34O2	1000495-78-7 25
3		2,4,4-Trimethyl-3-(3-methylbuta-...	206 C14H22O	097452-05-6 25
4		Benzo(a)acridine	229 C17H11N	000225-11-6 15
5		2-Butyl-3-methyl-5-(2-methylprop...	222 C15H26O	1000281-10-7 15



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129415.D
Acq On : 28 Jul 2022 18:38
Operator : CG\JU
Sample : N3895-18
Misc :
ALS Vial : 7 Sample Multiplier: 1

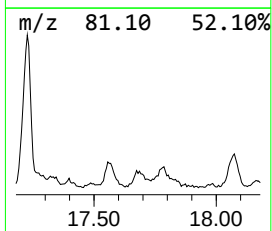
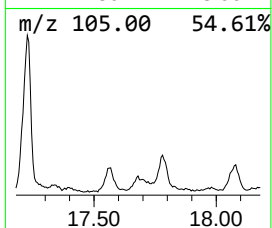
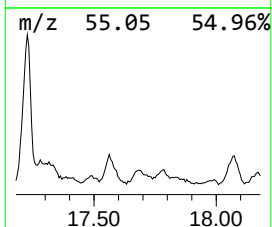
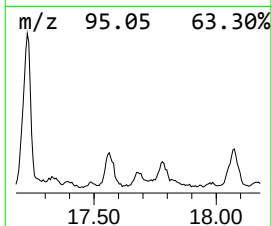
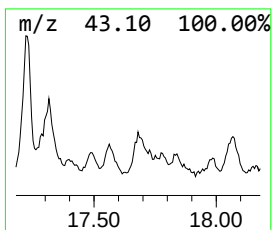
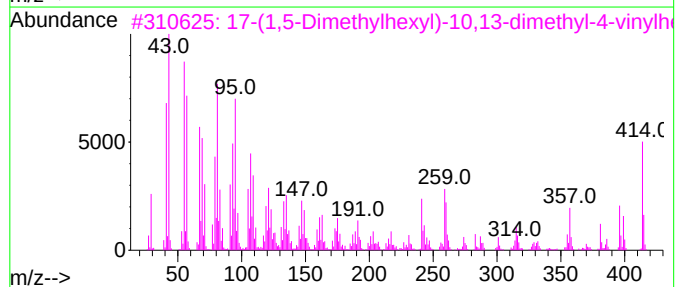
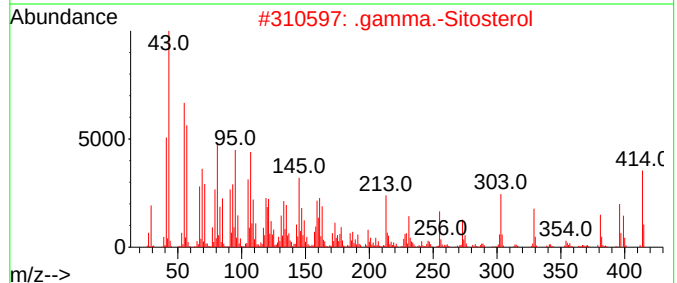
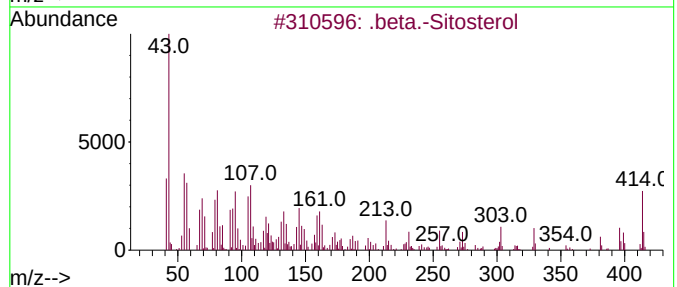
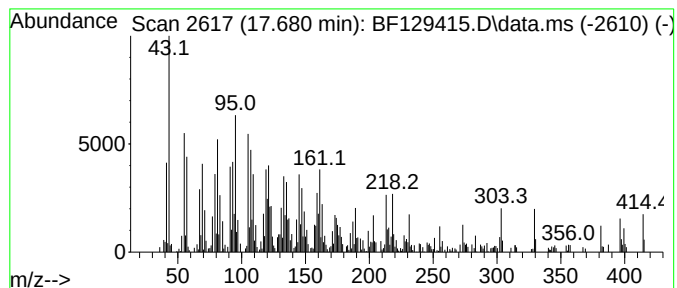
Instrument :
BNA_F
ClientSampleId :
RVE-56

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 .beta.-Sitosterol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.680	11.40 ng	730669	Perylene-d12	15.551	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol	414	C29H50O	000083-46-5	99
2	.gamma.-Sitosterol	414	C29H50O	000083-47-6	89
3	17-(1,5-Dimethylhexyl)-10,13-dim...	414	C29H50O	1000210-86-9	64
4	Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	004651-51-8	60
5	(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	51



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129415.D
Acq On : 28 Jul 2022 18:38
Operator : CG\JU
Sample : N3895-18
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-56

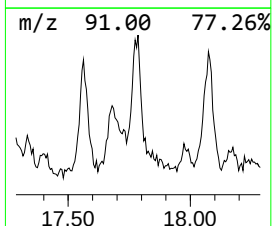
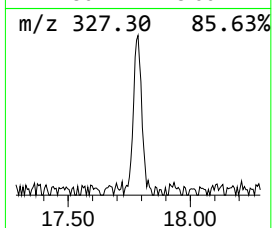
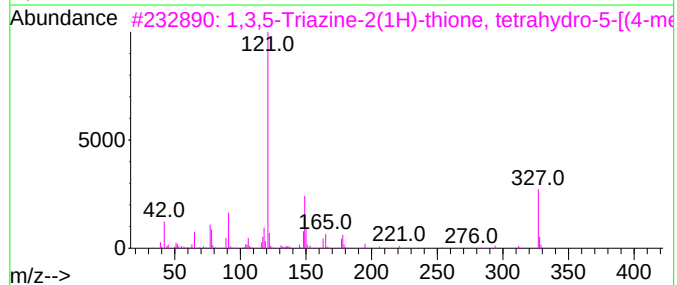
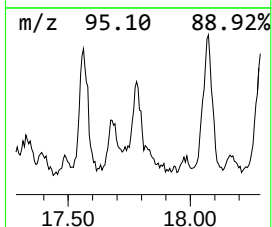
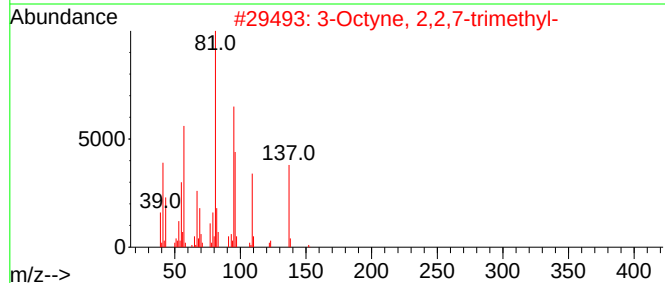
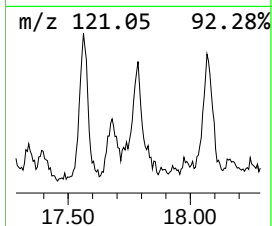
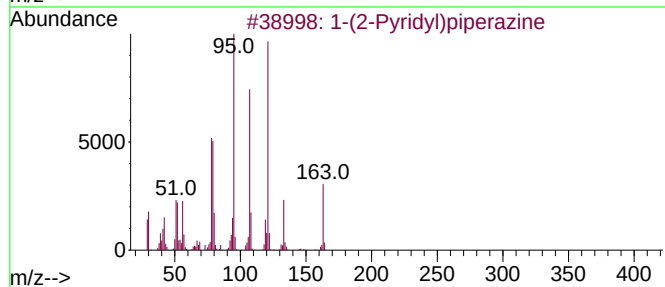
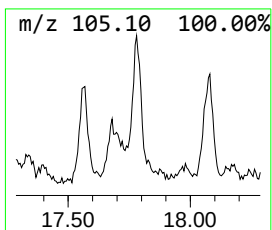
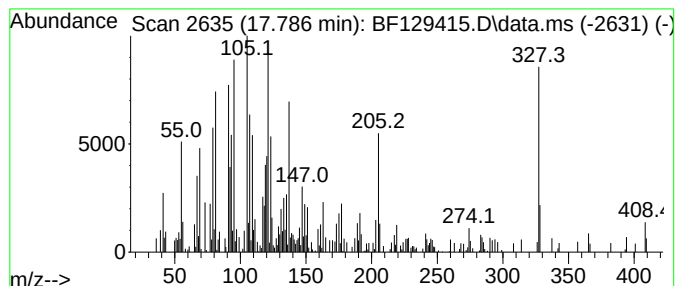
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown17.786 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.786	4.37 ng	279774	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(2-Pyridyl)piperazine		163	C9H13N3		034803-66-2	38
2	3-Octyne, 2,2,7-trimethyl-		152	C11H20		055402-13-6	25
3	1,3,5-Triazine-2(1H)-thione, tet...		327	C18H21N3OS		1000350-84-9	22
4	Benzamide, N-(4-cyano-5-methyl-2...		327	C14H9F4N3O2		1000310-19-1	22
5	Benzamide, N-(4-cyano-5-methyl-2...		327	C14H9F4N3O2		1000310-13-0	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129415.D
Acq On : 28 Jul 2022 18:38
Operator : CG\JU
Sample : N3895-18
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-56

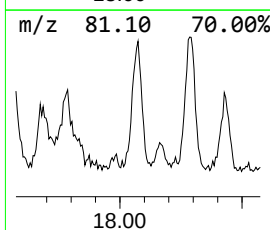
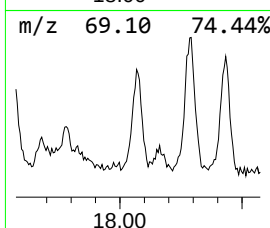
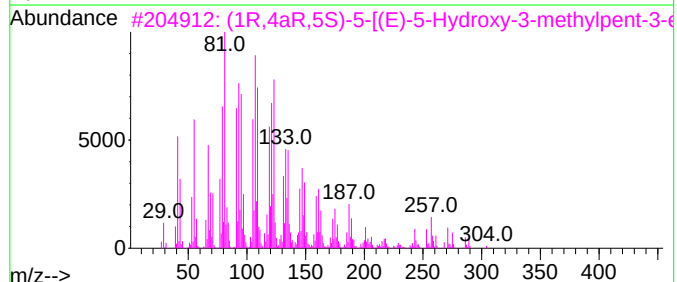
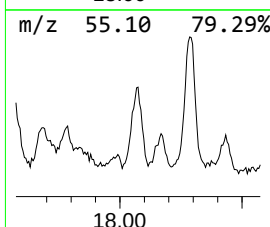
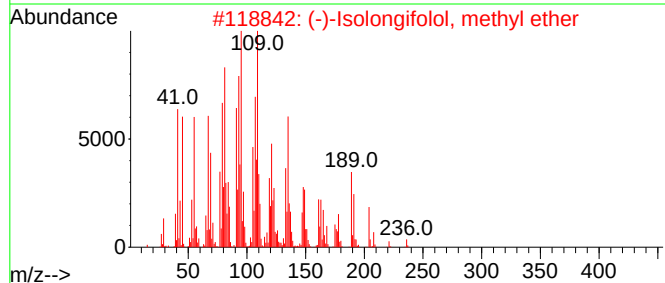
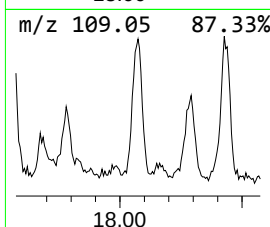
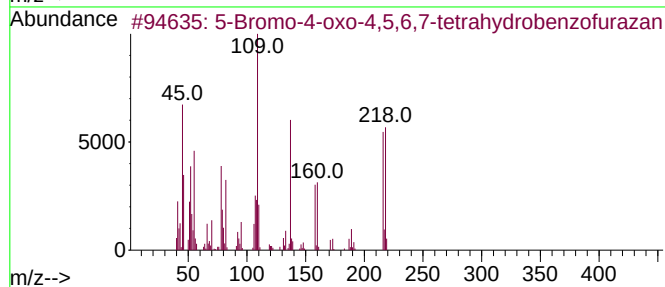
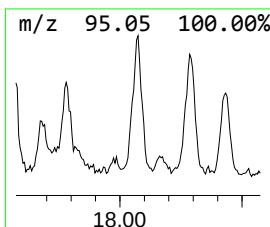
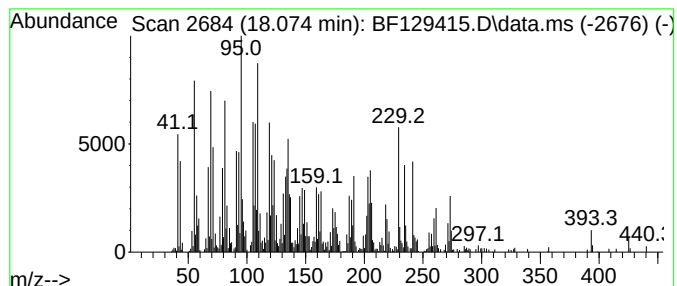
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 unknown18.074 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.074	16.90 ng	1082830	Perylene-d12	15.551

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	91
2		(-)-Isolongifolol, methyl ether	236	C16H28O	1000333-80-8	41
3		(1R,4aR,5S)-5-[(E)-5-Hydroxy-3-m...	304	C20H32O2	1214984-94-7	38
4		2-(4-Fluorobenzyl)-2-azaspiro[4...	261	C15H16FN02	1000332-10-7	35
5		4-(1,3,3-Trimethyl-bicyclo[4.1.0...	206	C14H22O	077143-31-8	20



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129415.D
Acq On : 28 Jul 2022 18:38
Operator : CG\JU
Sample : N3895-18
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-56

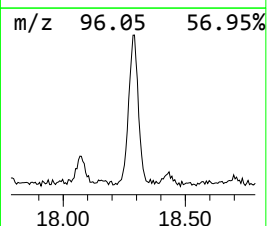
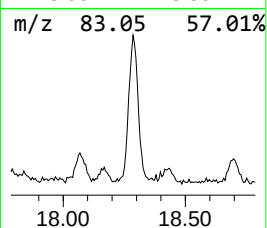
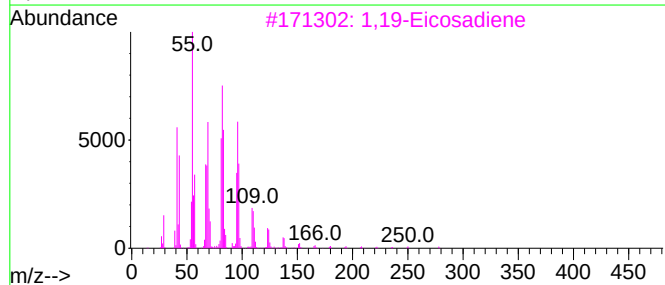
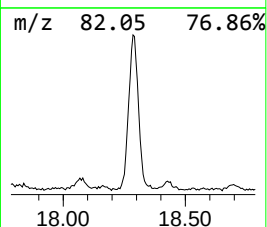
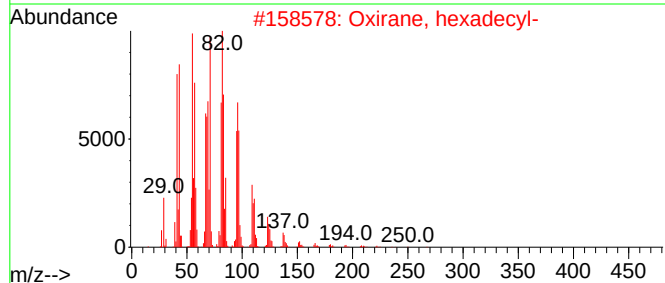
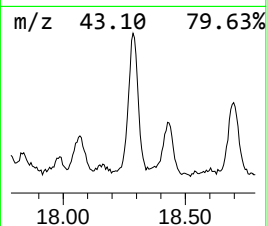
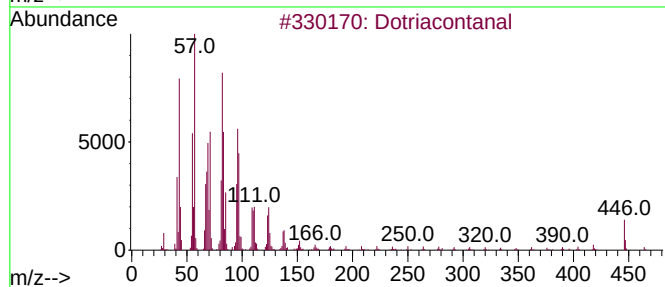
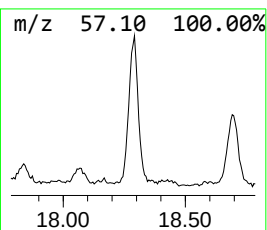
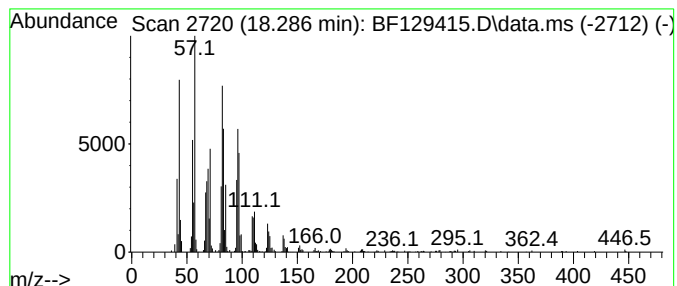
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Dotriacontanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.286	16.59 ng	1063100	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dotriacontanal	464	C32H64O	057878-00-9	91
2			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3			1,19-Eicosadiene	278	C20H38	014811-95-1	90
4			Octacosanal	408	C28H56O	022725-64-0	87
5			Octadecanal	268	C18H36O	000638-66-4	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129415.D
Acq On : 28 Jul 2022 18:38
Operator : CG\JU
Sample : N3895-18
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-56

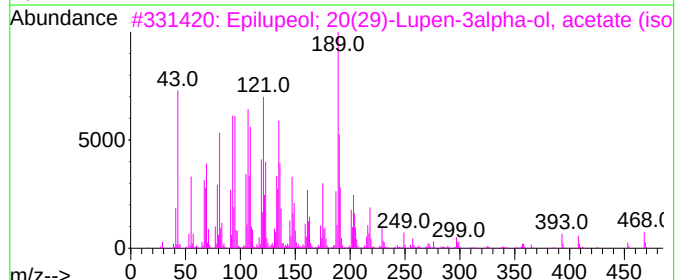
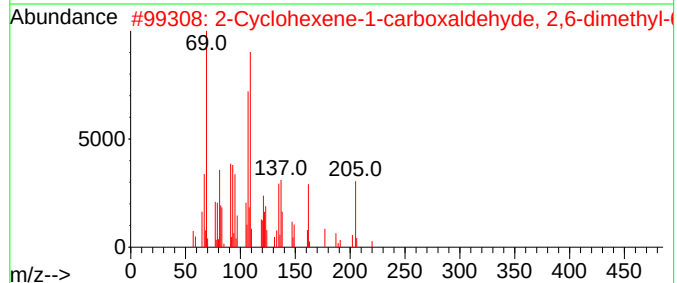
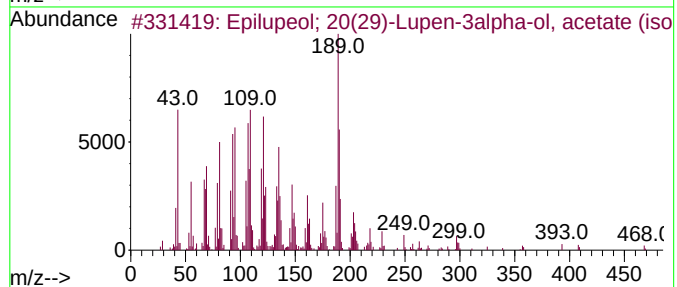
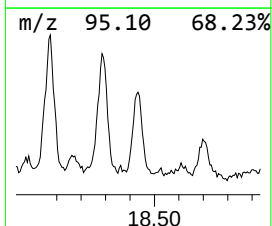
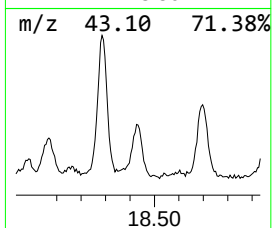
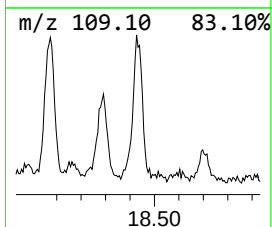
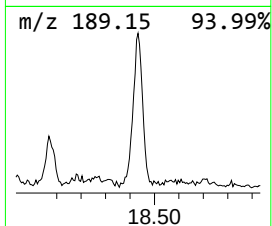
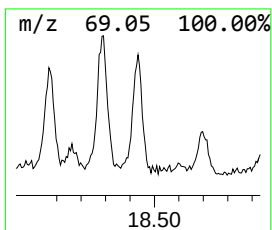
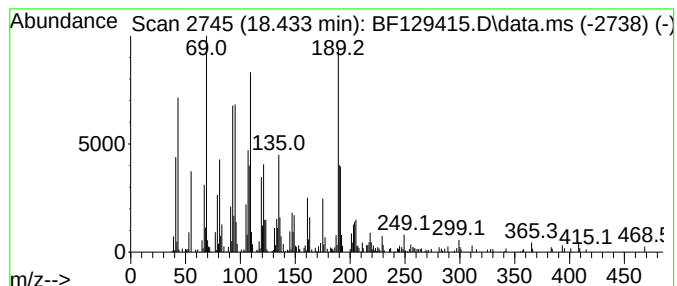
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown18.433 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.433	9.71 ng	622058	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Epilupeol; 20(29)-Lupen-3alpha-o...	468	C32H52O2	1010513-01-8	49
2			2-Cyclohexene-1-carboxaldehyde, ...	220	C15H24O	056772-07-7	38
3			Epilupeol; 20(29)-Lupen-3alpha-o...	468	C32H52O2	1000513-01-7	25
4			9-Methyltetracyclo[7.3.1.0(2.7)...]	204	C15H24	1000215-30-5	15
5			Panaginsene	204	C15H24	871660-96-7	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129415.D
Acq On : 28 Jul 2022 18:38
Operator : CG\JU
Sample : N3895-18
Misc :
ALS Vial : 7 Sample Multiplier: 1

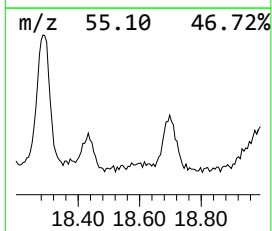
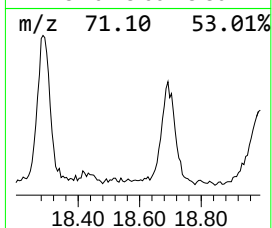
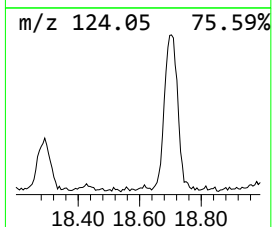
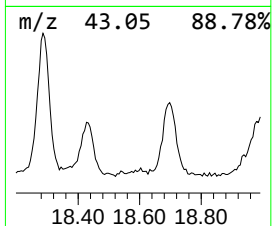
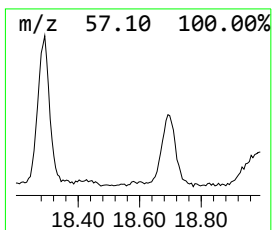
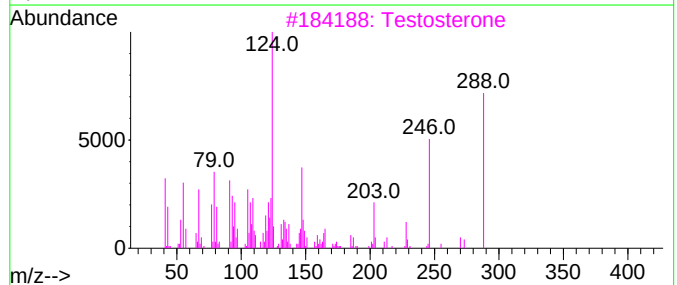
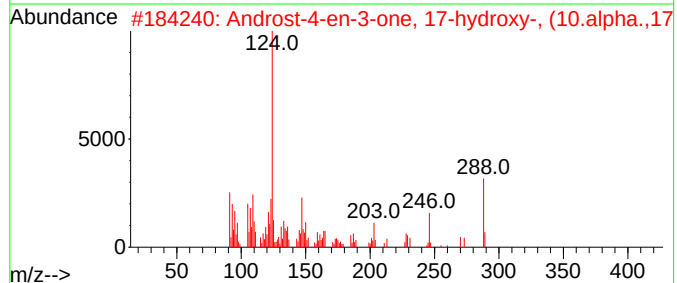
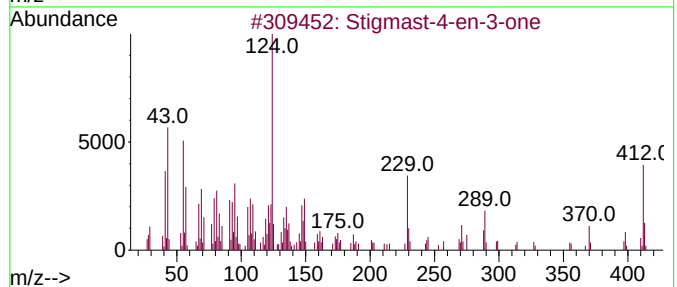
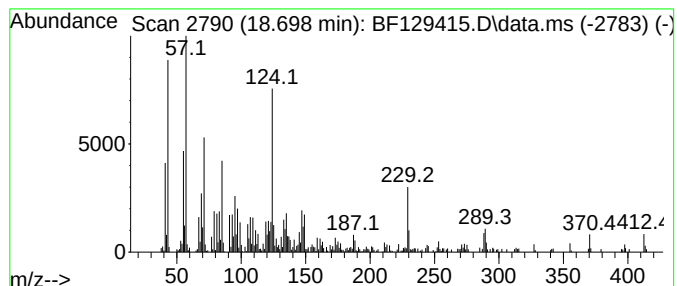
Instrument :
BNA_F
ClientSampleId :
RVE-56

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Stigmast-4-en-3-one Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.698	10.90 ng	698535	Perylene-d12		15.551	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Stigmast-4-en-3-one		412	C29H48O	001058-61-3	70
2	Androst-4-en-3-one, 17-hydroxy-,...		288	C19H28O2	000604-39-7	64
3	Testosterone		288	C19H28O2	000058-22-0	58
4	Heptacosane, 1-chloro-		414	C27H55Cl	062016-79-9	55
5	3-Octenoic acid, undecyl ester		296	C19H36O2	1000406-13-1	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129415.D
Acq On : 28 Jul 2022 18:38
Operator : CG\JU
Sample : N3895-18
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-56

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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
Coumarin	9.675	4.3	ng	412216	3	9.922	1898190	20.0
n-Hexadecanoic ...	11.933	5.4	ng	458629	4	11.416	1699450	20.0
Heptafluorobuty...	13.904	16.2	ng	868076	5	14.057	1068960	20.0
Tridecane, 6-pr...	14.510	4.5	ng	237939	5	14.057	1068960	20.0
1,19-Eicosadiene	14.968	8.5	ng	544159	6	15.551	1281470	20.0
Eicosane	15.163	9.1	ng	581972	6	15.551	1281470	20.0
1-Nonadecene	15.221	13.5	ng	867159	6	15.551	1281470	20.0
Oxirane, hexade...	15.762	12.4	ng	792926	6	15.551	1281470	20.0
Heptadecane, 9-...	15.998	21.8	ng	1398750	6	15.551	1281470	20.0
Cyclotetracosane	16.092	9.3	ng	594756	6	15.551	1281470	20.0
Octadecanal	16.815	9.8	ng	629076	6	15.551	1281470	20.0
Heneicosane	17.121	21.1	ng	1348720	6	15.551	1281470	20.0
1,1,4a-Trimethy...	17.227	89.1	ng	5708140	6	15.551	1281470	20.0
5-Bromo-4-oxo-4...	17.562	15.9	ng	1020020	6	15.551	1281470	20.0
.beta.-Sitosterol	17.680	11.4	ng	730669	6	15.551	1281470	20.0
unknown17.786	17.786	4.4	ng	279774	6	15.551	1281470	20.0
unknown18.074	18.074	16.9	ng	1082830	6	15.551	1281470	20.0
Dotriacontanal	18.286	16.6	ng	1063100	6	15.551	1281470	20.0
unknown18.433	18.433	9.7	ng	622058	6	15.551	1281470	20.0
Stigmast-4-en-3...	18.698	10.9	ng	698535	6	15.551	1281470	20.0