

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
 Data File : BF138275.D
 Acq On : 20 Jun 2024 21:43
 Operator : CG\JU
 Sample : P2977-02
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OSTL-A2

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-BF061224.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138275.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	12	18	23	rVB	2636074	3215908	52.88%	6.669%
2	3.399	220	223	240	rBV	59674	129200	2.12%	0.268%
3	5.104	510	513	524	rVB	276371	308259	5.07%	0.639%
4	5.504	576	581	584	rBV	4941892	4716258	77.56%	9.781%
5	5.828	632	636	643	rBV	81001	72320	1.19%	0.150%
6	6.510	746	752	755	rBV	4793600	4736962	77.90%	9.824%
7	6.881	812	815	819	rVB	2132620	1818235	29.90%	3.771%
8	7.445	906	911	914	rBV	3416006	3085115	50.73%	6.398%
9	7.692	950	953	957	rBV	184939	156485	2.57%	0.325%
10	7.969	997	1000	1004	rBV	124598	101394	1.67%	0.210%
11	8.163	1029	1033	1036	rBV	2959936	2441219	40.14%	5.063%
12	8.475	1082	1086	1096	rBV	185820	230412	3.79%	0.478%
13	9.239	1211	1216	1219	rBV	7326912	6081094	100.00%	12.611%
14	9.669	1285	1289	1298	rVB	949512	769606	12.66%	1.596%
15	9.916	1327	1331	1335	rBV	3208337	2842092	46.74%	5.894%
16	10.016	1342	1348	1355	rBV	72506	103772	1.71%	0.215%
17	10.704	1461	1465	1479	rVB	4037082	3631211	59.71%	7.531%
18	11.404	1580	1584	1587	rBV	3255618	2566532	42.21%	5.323%
19	11.927	1670	1673	1682	rBV	528432	493507	8.12%	1.023%
20	12.616	1786	1790	1792	rBV	90840	85694	1.41%	0.178%
21	12.710	1803	1806	1815	rBV	83228	102149	1.68%	0.212%
22	12.986	1849	1853	1857	rBV	5459513	4745480	78.04%	9.841%
23	13.921	2003	2012	2027	rBV4	127054	498672	8.20%	1.034%
24	14.039	2028	2032	2035	rBV	1915898	1622776	26.69%	3.365%
25	14.568	2116	2122	2126	rBV6	56589	132145	2.17%	0.274%
26	14.898	2174	2178	2182	rBV	227942	215870	3.55%	0.448%
27	14.968	2186	2190	2196	rVV	222151	216239	3.56%	0.448%
28	15.162	2219	2223	2227	rBV	105818	117664	1.93%	0.244%
29	15.245	2230	2237	2250	rBV3	102684	367229	6.04%	0.762%
30	15.515	2277	2283	2287	rBV	1411187	1835716	30.19%	3.807%
31	15.757	2319	2324	2331	rBV	152188	209526	3.45%	0.435%
32	15.992	2360	2364	2371	rVB2	94280	136034	2.24%	0.282%
33	16.115	2377	2385	2403	rBV5	74411	334801	5.51%	0.694%
34	16.809	2498	2503	2511	rVB5	51029	100002	1.64%	0.207%

Sum of corrected areas: 48219578

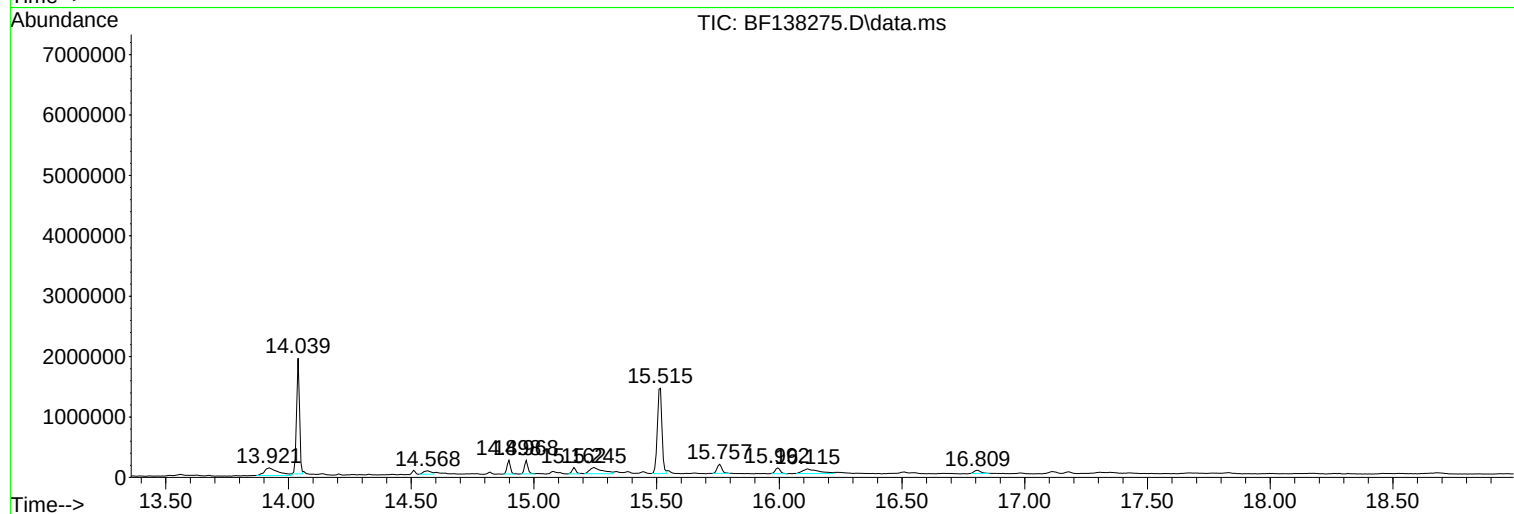
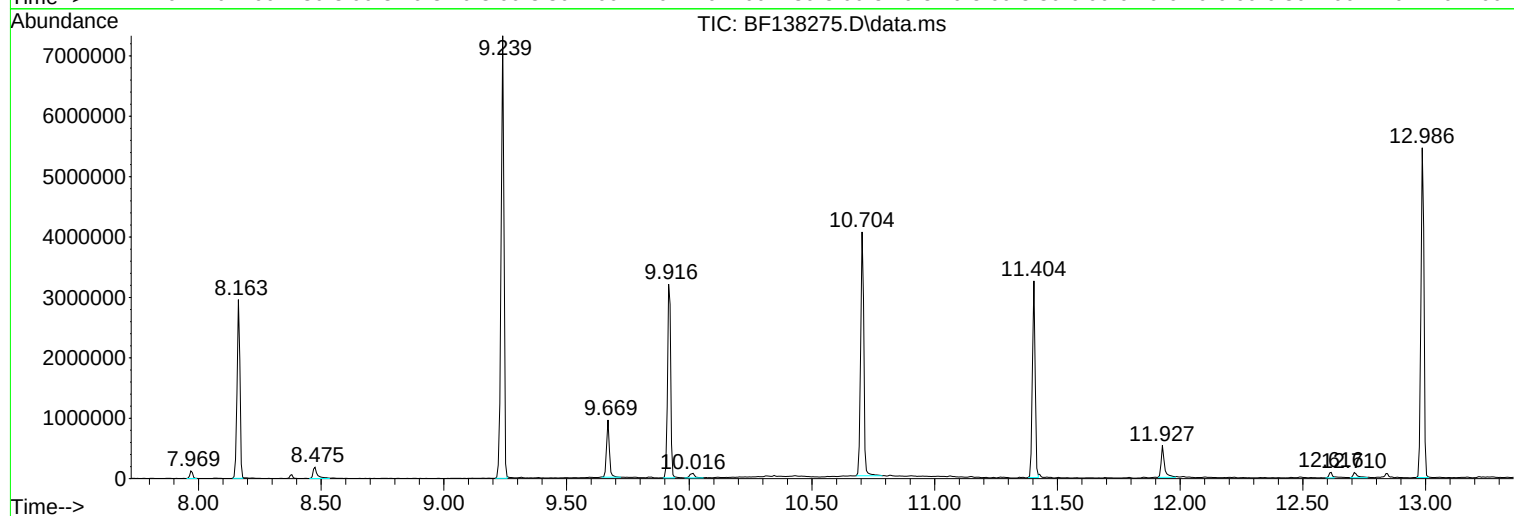
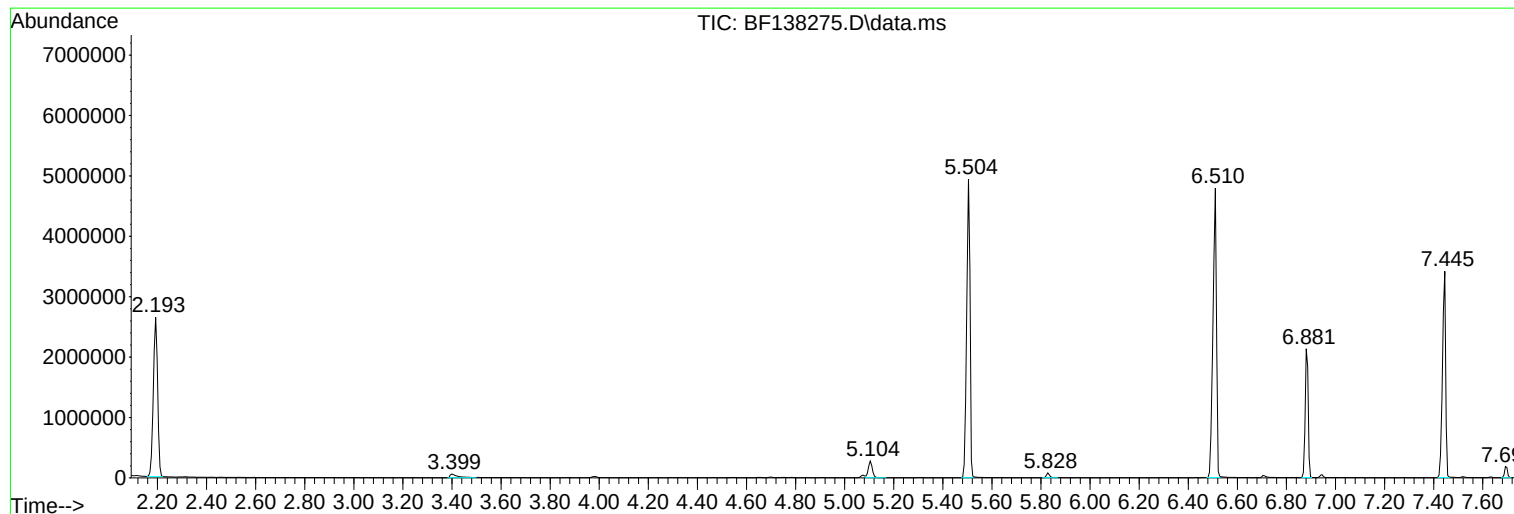
Instrument :
BNA_F
ClientSampleId :
OSTL-A2

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
Data File : BF138275.D
Acq On : 20 Jun 2024 21:43
Operator : CG\JU
Sample : P2977-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-A2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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\BF062024\
Data File : BF138275.D
Acq On : 20 Jun 2024 21:43
Operator : CG\JU
Sample : P2977-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-A2

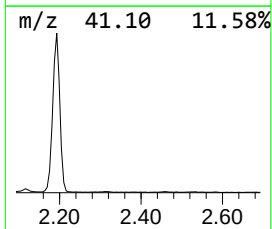
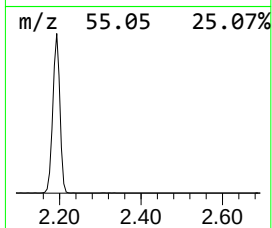
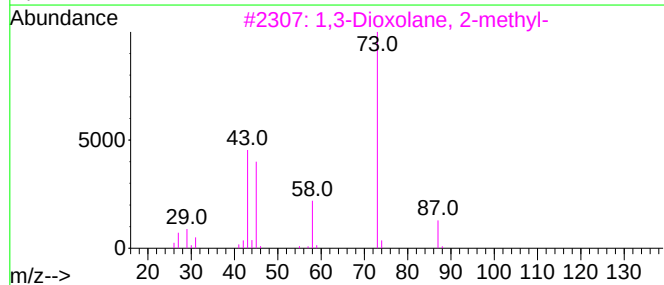
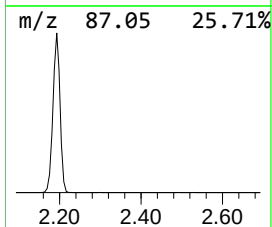
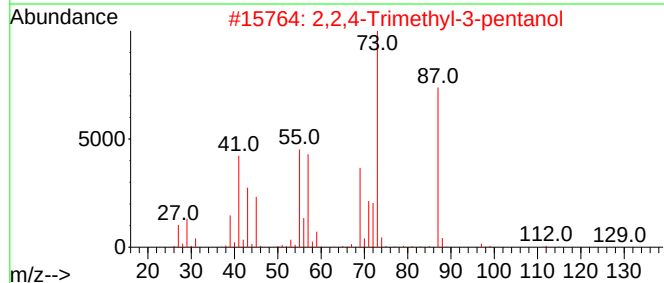
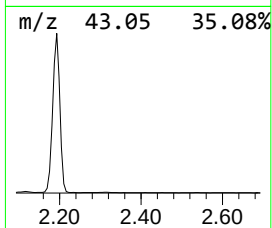
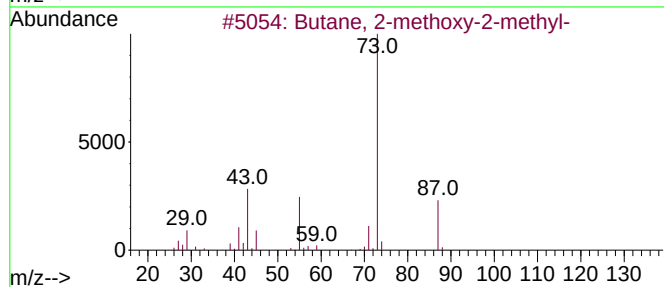
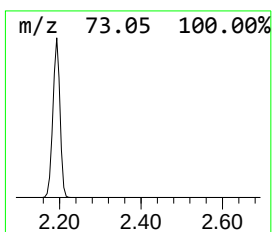
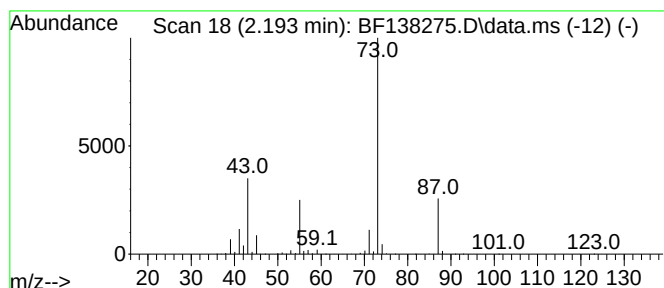
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.193	35.37 ng	3215910	1,4-Dichlorobenzene-d4	6.881

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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
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\BF062024\
Data File : BF138275.D
Acq On : 20 Jun 2024 21:43
Operator : CG\JU
Sample : P2977-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-A2

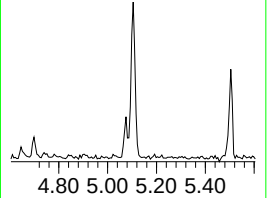
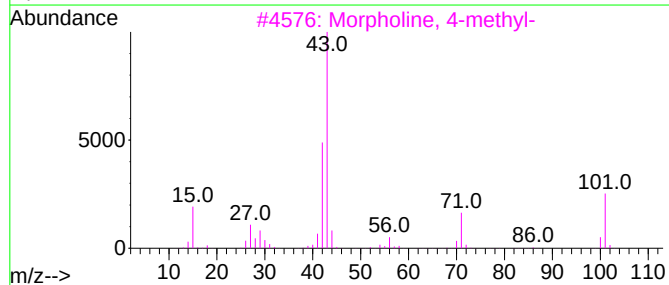
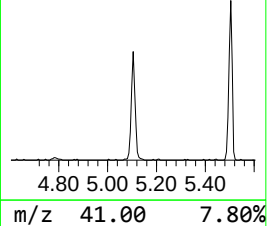
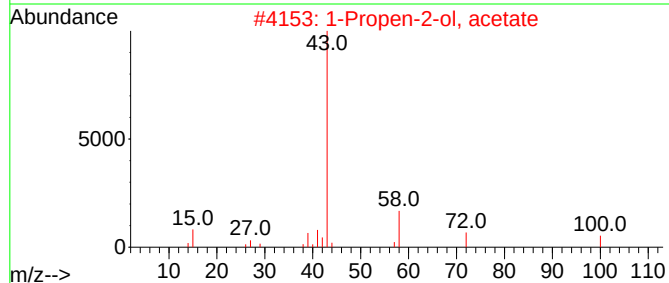
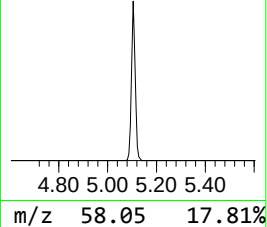
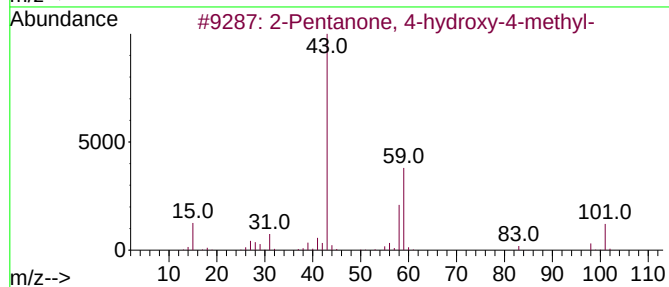
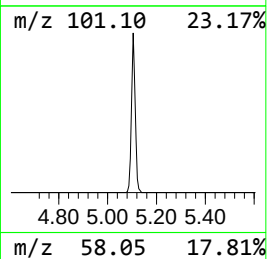
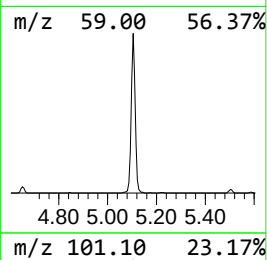
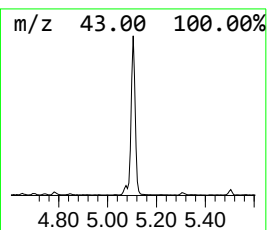
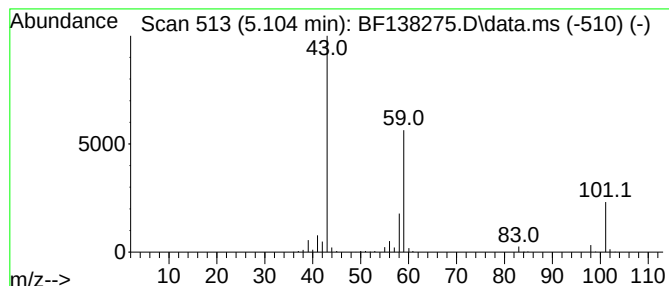
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	3.39 ng	308259	1,4-Dichlorobenzene-d4	6.881

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
Data File : BF138275.D
Acq On : 20 Jun 2024 21:43
Operator : CG\JU
Sample : P2977-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-A2

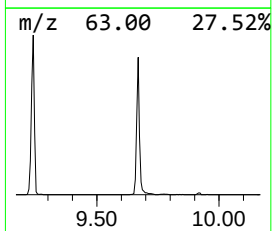
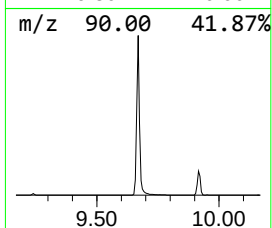
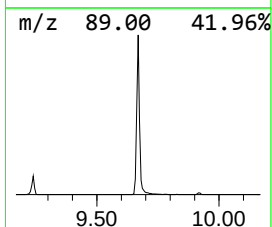
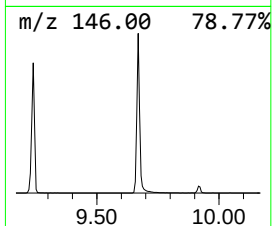
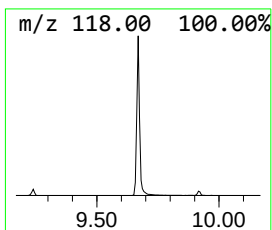
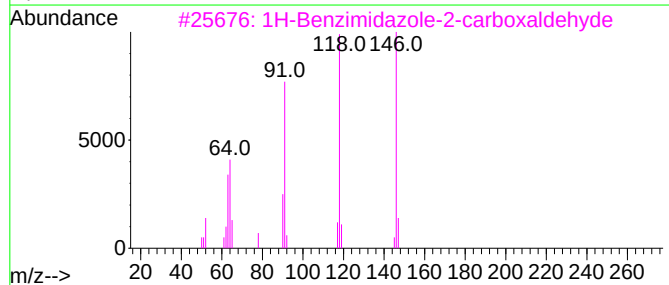
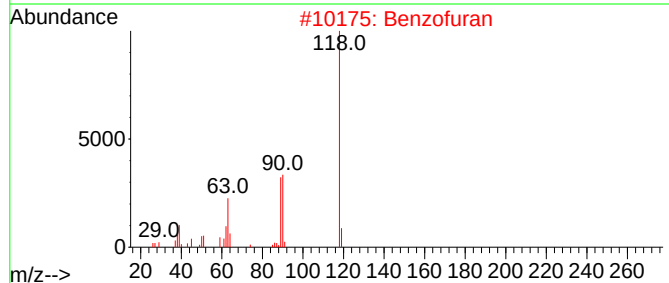
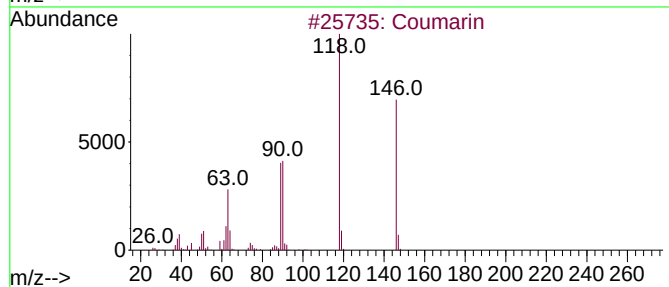
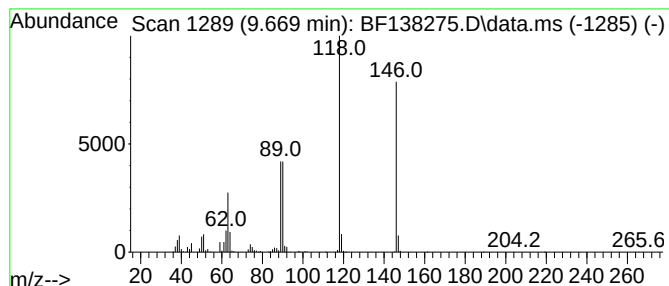
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Coumarin Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.669	5.42 ng	769606	Acenaphthene-d10	9.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Coumarin	146	C9H6O2	000091-64-5	98
2			Benzofuran	118	C8H6O	000271-89-6	96
3			1H-Benzimidazole-2-carboxaldehyde	146	C8H6N2O	003314-30-5	58
4			Phthalazin-1-one	146	C8H6N2O	000119-39-1	58
5			1(2H)-Naphthalenone, 3,4-dihydro-	146	C10H10O	000529-34-0	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
Data File : BF138275.D
Acq On : 20 Jun 2024 21:43
Operator : CG\JU
Sample : P2977-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

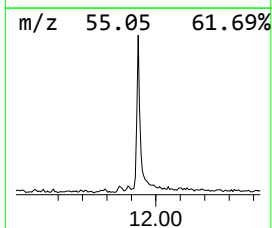
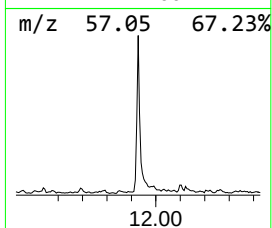
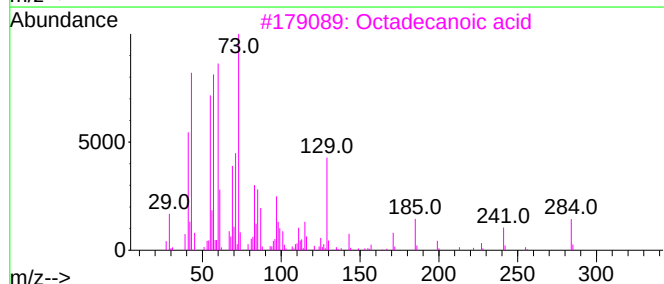
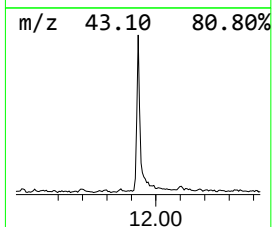
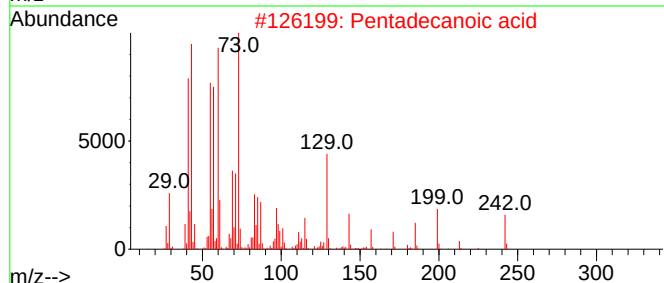
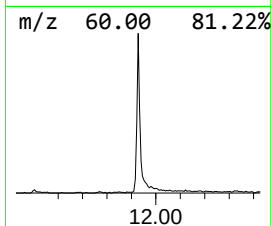
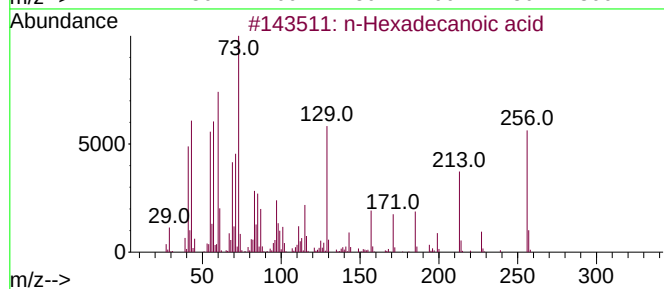
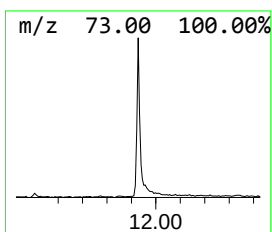
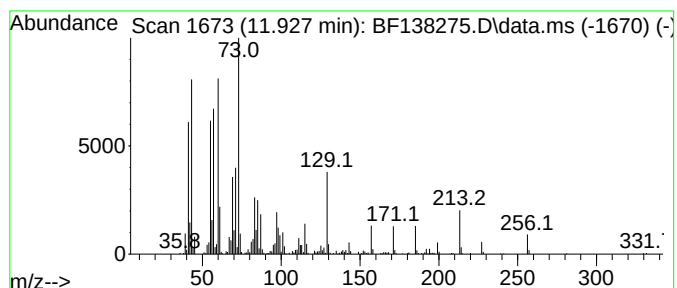
Instrument :
BNA_F
ClientSampleId :
OSTL-A2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.927	3.85 ng	493507	Phenanthrene-d10	11.404	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Octadecanoic acid	284	C18H36O2	000057-11-4	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
Data File : BF138275.D
Acq On : 20 Jun 2024 21:43
Operator : CG\JU
Sample : P2977-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-A2

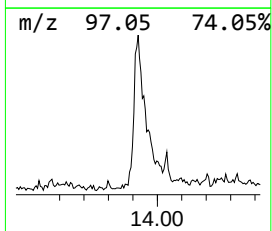
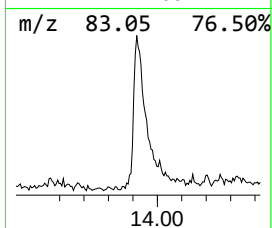
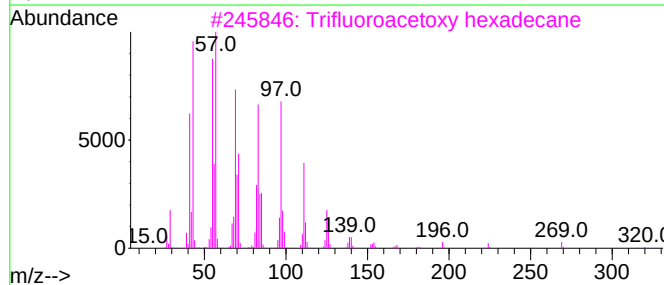
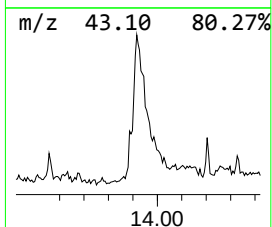
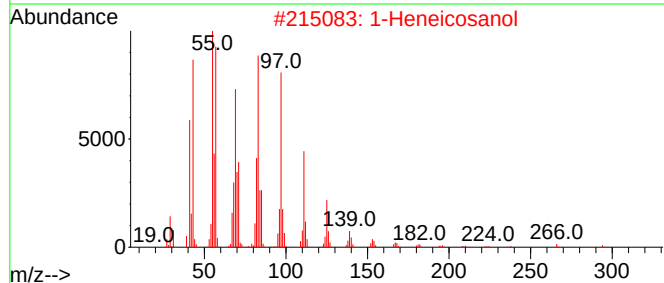
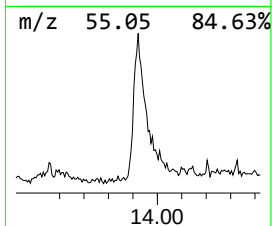
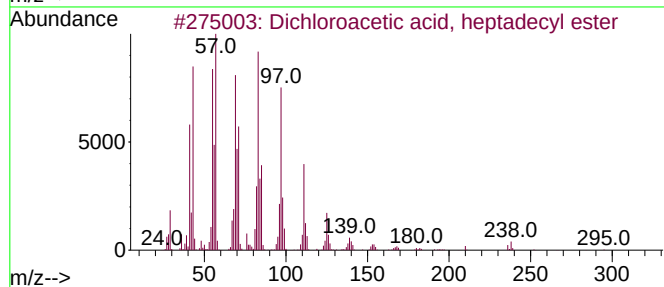
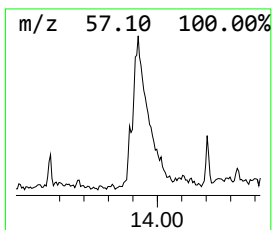
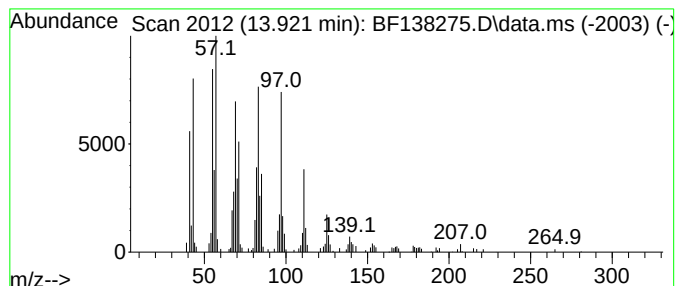
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Dichloroacetic acid, heptad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	6.15 ng	498672	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2			1-Heneicosanol	312	C21H44O	015594-90-8	95
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
4			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
Data File : BF138275.D
Acq On : 20 Jun 2024 21:43
Operator : CG\JU
Sample : P2977-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-A2

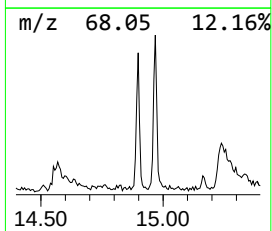
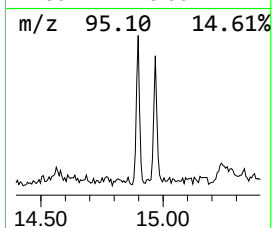
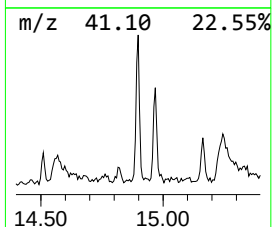
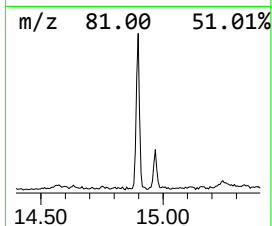
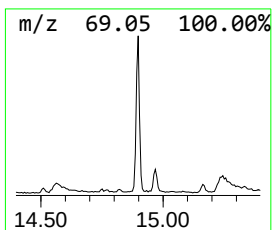
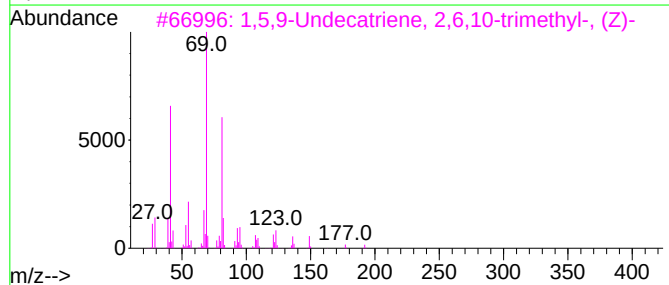
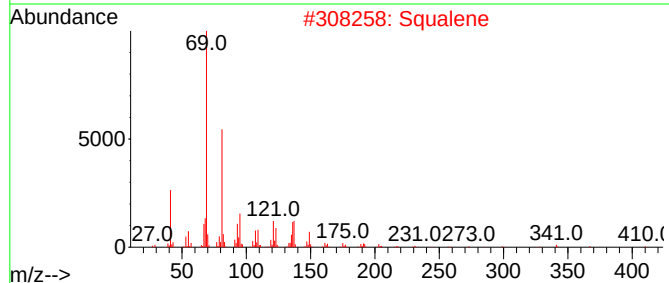
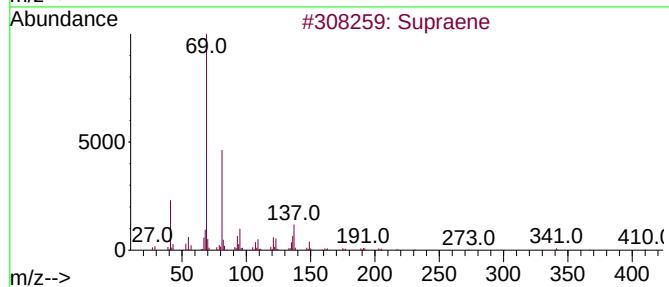
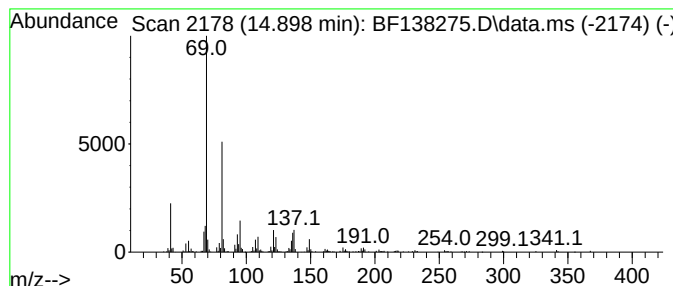
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.898	2.35 ng	215870	Perylene-d12	15.515

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			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	86
4			2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	53
5			2,6-Octadiene, 4,5-dimethyl-	138	C10H18	018476-57-8	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
Data File : BF138275.D
Acq On : 20 Jun 2024 21:43
Operator : CG\JU
Sample : P2977-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-A2

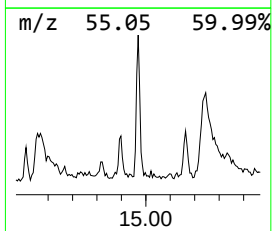
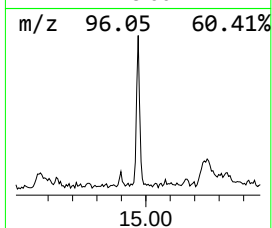
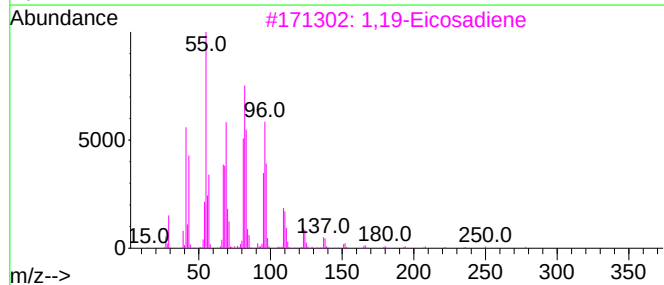
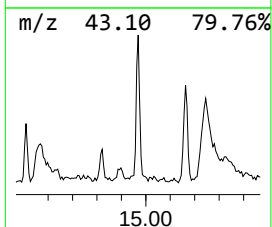
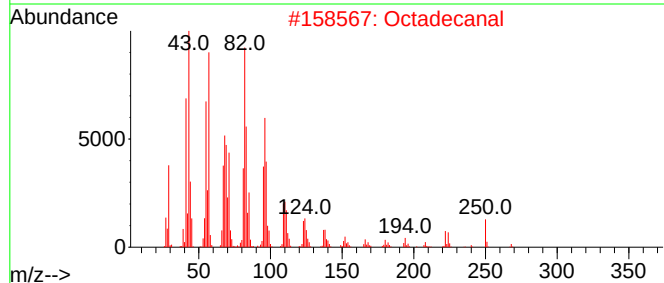
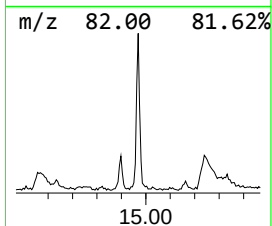
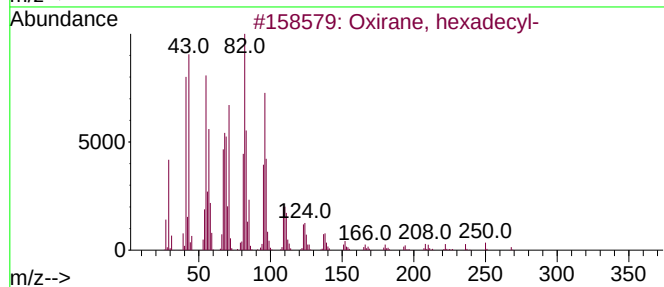
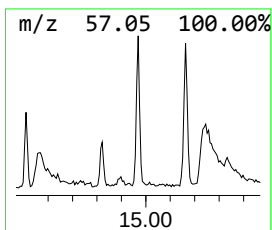
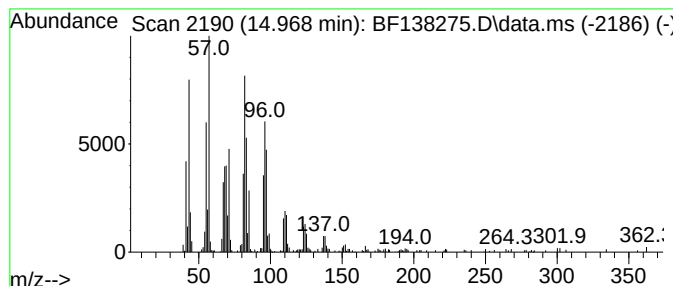
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Oxirane, hexadecyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.968	2.36 ng	216239	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	95
2			Octadecanal	268	C18H36O	000638-66-4	95
3			1,19-Eicosadiene	278	C20H38	014811-95-1	94
4			Eicosanal	296	C20H40O	002400-66-0	90
5			Tetracosanal	352	C24H48O	057866-08-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
Data File : BF138275.D
Acq On : 20 Jun 2024 21:43
Operator : CG\JU
Sample : P2977-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-A2

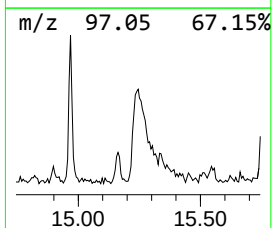
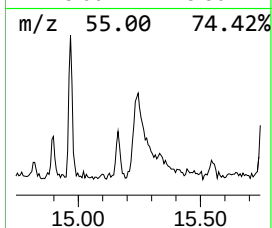
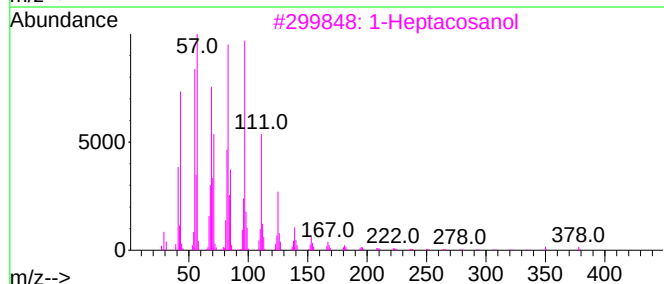
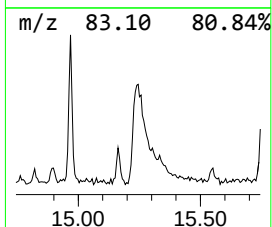
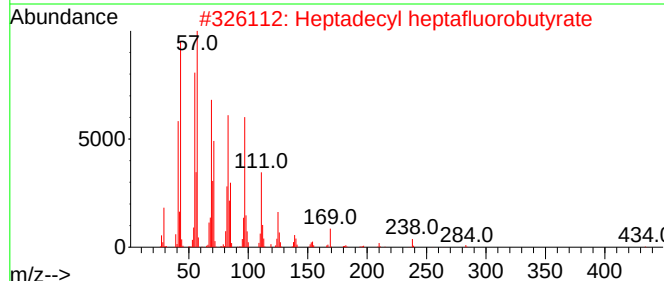
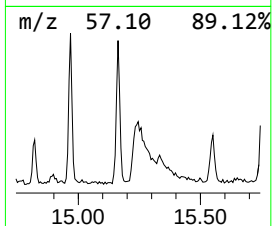
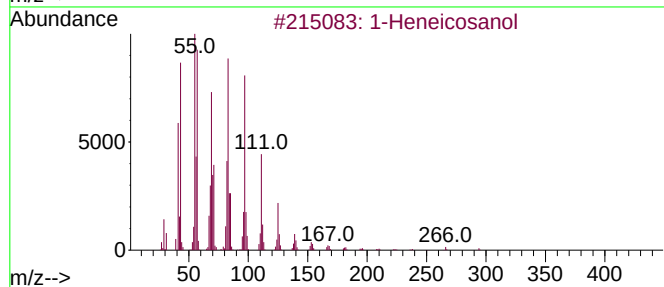
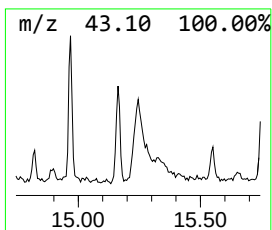
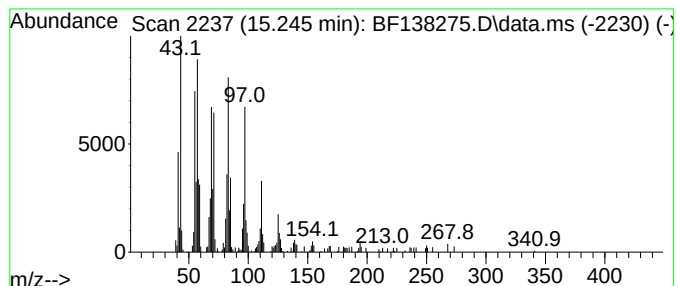
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.245	4.00 ng	367229	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	93
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3			1-Heptacosanol	396	C27H56O	002004-39-9	91
4			Triacontan-15-ol	438	C30H62O	031849-26-0	87
5			1-Hexacosanol	382	C26H54O	000506-52-5	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
Data File : BF138275.D
Acq On : 20 Jun 2024 21:43
Operator : CG\JU
Sample : P2977-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-A2

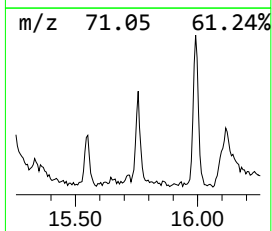
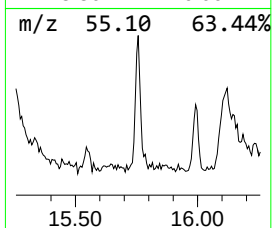
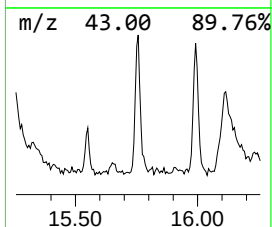
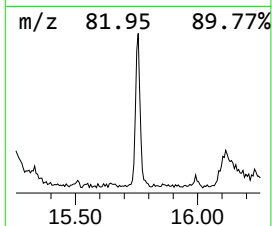
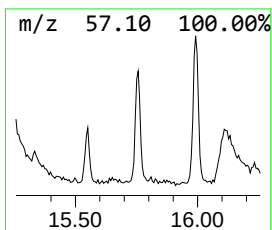
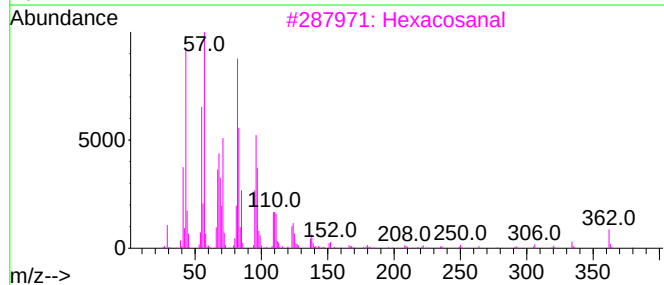
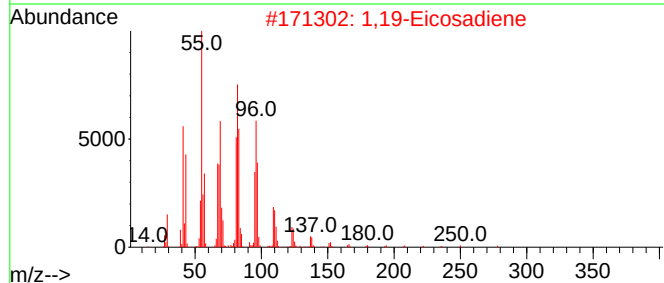
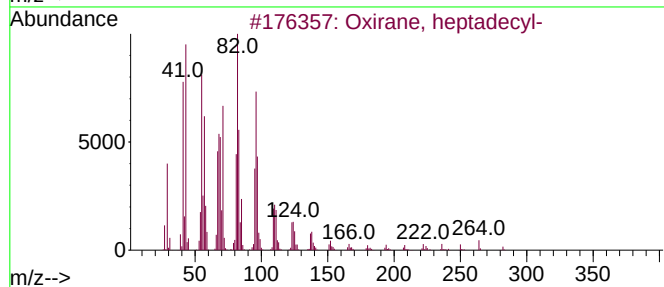
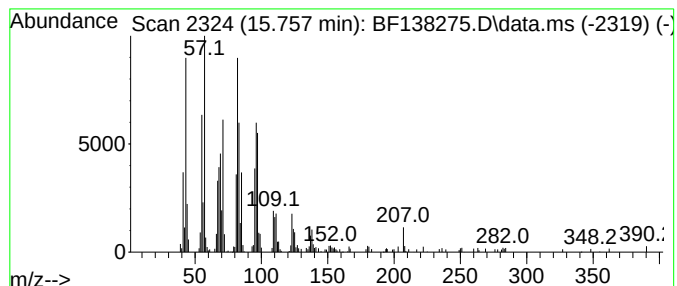
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Oxirane, heptadecyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.757	2.28 ng	209526	Perylene-d12	15.515

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	94
2		1,19-Eicosadiene	278	C20H38	014811-95-1	93
3		Hexacosanal	380	C26H52O	026627-85-0	87
4		Eicosanal	296	C20H40O	002400-66-0	87
5		Octadecanal	268	C18H36O	000638-66-4	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
Data File : BF138275.D
Acq On : 20 Jun 2024 21:43
Operator : CG\JU
Sample : P2977-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-A2

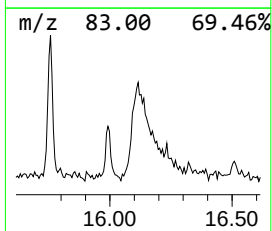
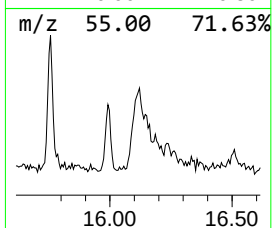
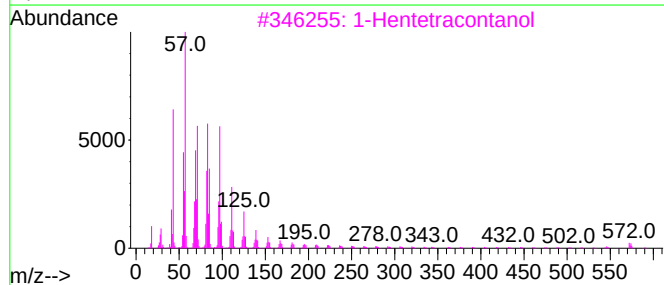
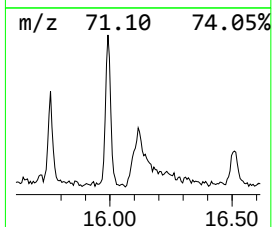
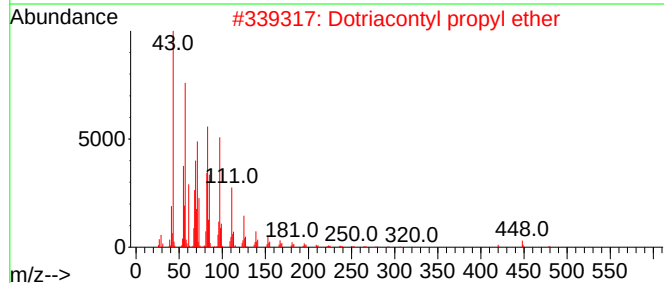
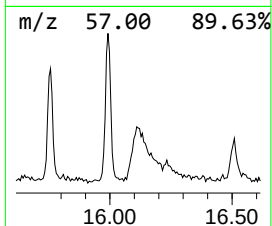
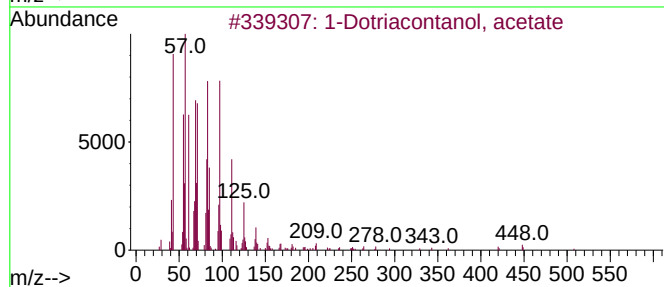
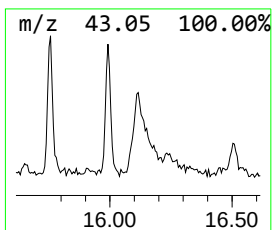
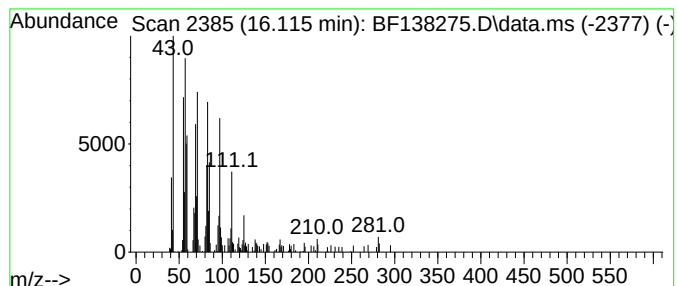
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Dotriacontanol, acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.115	3.65 ng	334801	Perylene-d12	15.515

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Dotriacontanol, acetate	509	C34H68O2	023811-94-1	76
2		Dotriacontyl propyl ether	509	C35H72O	1000406-28-7	68
3		1-Hentetracontanol	593	C41H84O	040710-42-7	68
4		Butyl tetratriacontyl ether	551	C38H78O	1000406-41-4	62
5		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
Data File : BF138275.D
Acq On : 20 Jun 2024 21:43
Operator : CG\JU
Sample : P2977-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-A2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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...	2.193	35.4	ng	3215910	1	6.881	1818240	20.0
2-Pentanone, 4-...	5.104	3.4	ng	308259	1	6.881	1818240	20.0
Coumarin	9.669	5.4	ng	769606	3	9.916	2842090	20.0
n-Hexadecanoic ...	11.927	3.9	ng	493507	4	11.404	2566530	20.0
Dichloroacetic ...	13.921	6.2	ng	498672	5	14.039	1622780	20.0
Supraene	14.898	2.4	ng	215870	6	15.515	1835720	20.0
Oxirane, hexade...	14.968	2.4	ng	216239	6	15.515	1835720	20.0
1-Heneicosanol	15.245	4.0	ng	367229	6	15.515	1835720	20.0
Oxirane, heptad...	15.757	2.3	ng	209526	6	15.515	1835720	20.0
1-Dotriacontano...	16.115	3.6	ng	334801	6	15.515	1835720	20.0