

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061024\
 Data File : BF138176.D
 Acq On : 10 Jun 2024 17:09
 Operator : CG\JU
 Sample : P2784-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WCS-TPD

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-BF060524.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138176.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	24	rBV	4518351	5545831	66.04%	8.335%
2	3.422	220	227	251	rBV	332715	792349	9.44%	1.191%
3	5.110	511	514	523	rVB	309150	340198	4.05%	0.511%
4	5.516	577	583	586	rBV	6018085	6013952	71.61%	9.039%
5	6.440	733	740	748	rBV2	39971	87895	1.05%	0.132%
6	6.516	748	753	756	rBV	6067999	6196043	73.78%	9.312%
7	6.716	784	787	793	rBV	450037	379866	4.52%	0.571%
8	6.893	814	817	821	rVB	2659533	2265259	26.97%	3.405%
9	7.457	908	913	916	rBV	4223567	3698407	44.04%	5.559%
10	7.704	952	955	959	rVB	156479	128414	1.53%	0.193%
11	8.175	1031	1035	1038	rBV	3797904	2993355	35.65%	4.499%
12	8.487	1084	1088	1097	rBV	533188	485906	5.79%	0.730%
13	9.251	1214	1218	1221	rBV	9232767	7432657	88.51%	11.171%
14	9.928	1330	1333	1337	rVB	3839668	3383377	40.29%	5.085%
15	10.033	1345	1351	1354	rBV	6563226	8397629	100.00%	12.621%
16	10.716	1463	1467	1470	rBV	4587962	3780575	45.02%	5.682%
17	11.416	1582	1586	1589	rBV	3889499	3052457	36.35%	4.588%
18	11.945	1671	1676	1686	rBV2	482277	523382	6.23%	0.787%
19	12.516	1767	1773	1781	rVB2	94753	108418	1.29%	0.163%
20	12.727	1805	1809	1816	rBV	188096	201607	2.40%	0.303%
21	12.998	1851	1855	1859	rBV	6250204	5537498	65.94%	8.323%
22	13.480	1933	1937	1951	rBV	565336	678544	8.08%	1.020%
23	13.904	2005	2009	2018	rBV	144024	211571	2.52%	0.318%
24	14.051	2030	2034	2046	rBV	2403571	2049166	24.40%	3.080%
25	14.916	2177	2181	2186	rBV	251412	244133	2.91%	0.367%
26	15.527	2279	2285	2291	rBV	1661269	2006755	23.90%	3.016%

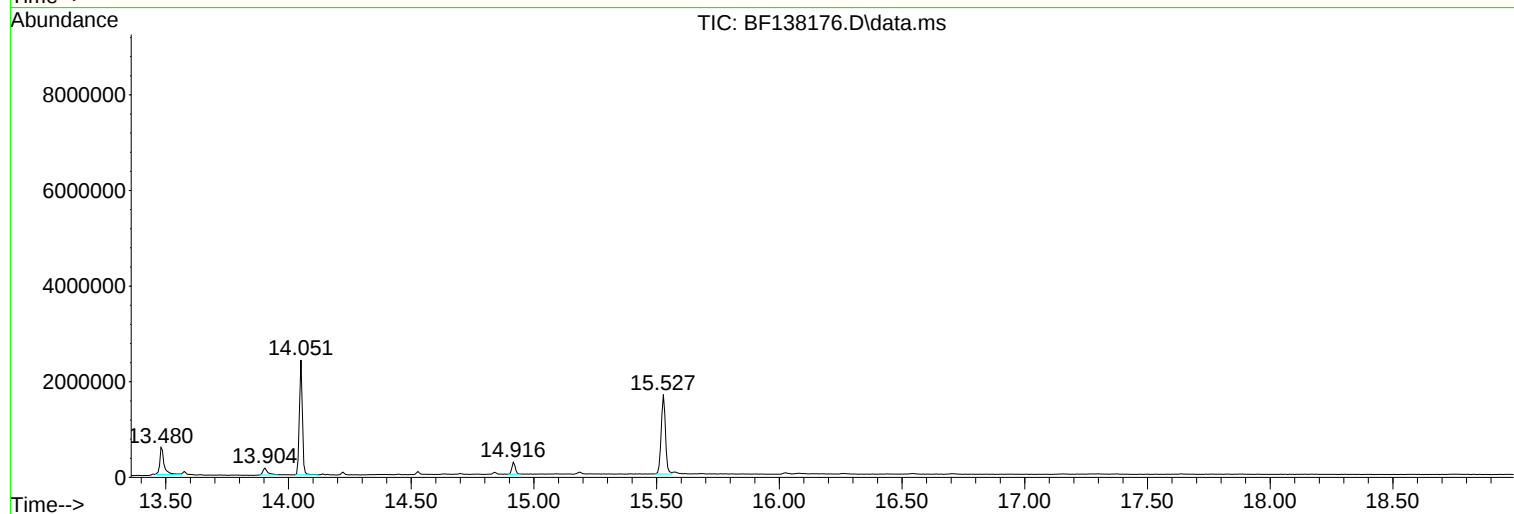
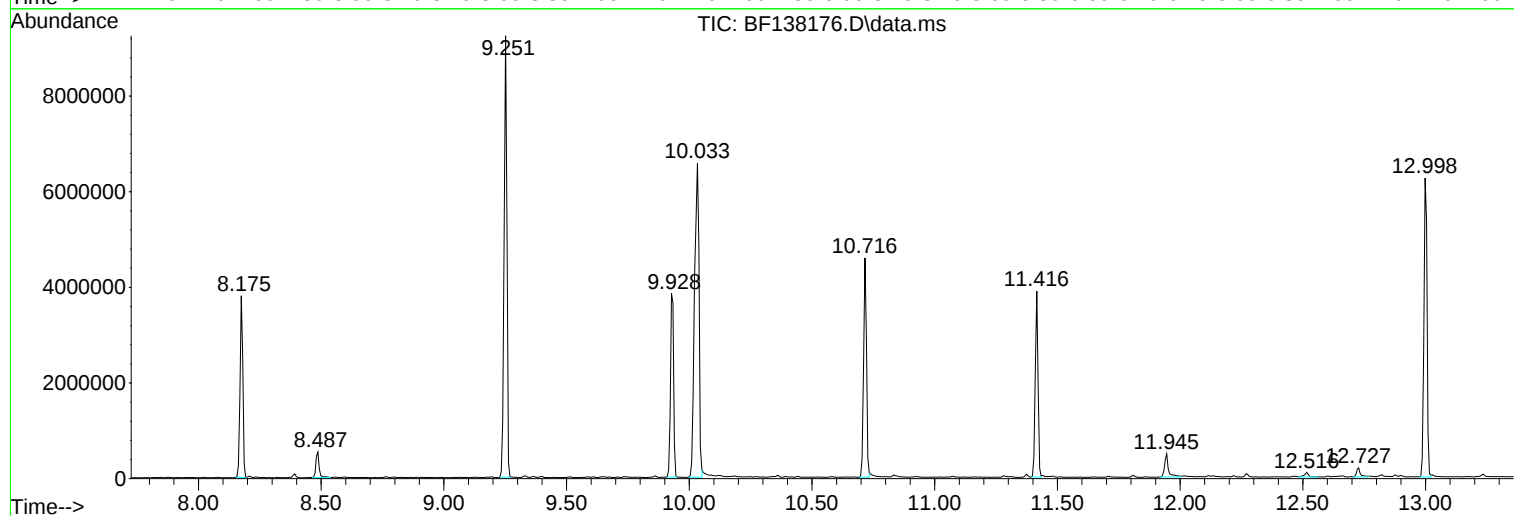
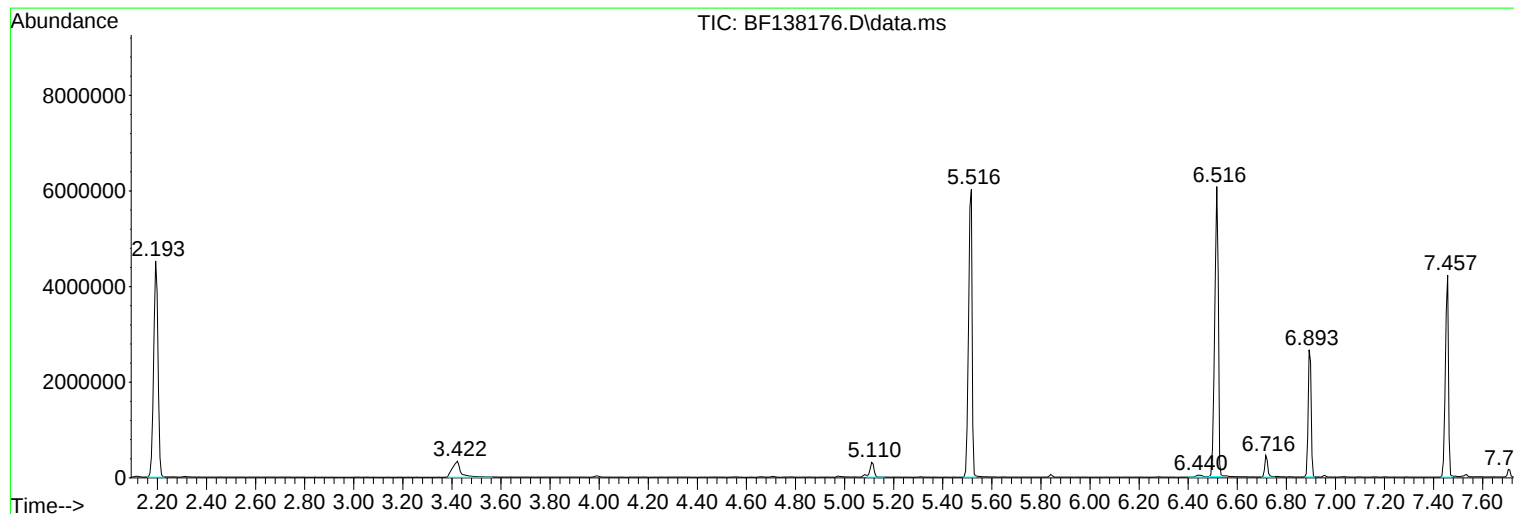
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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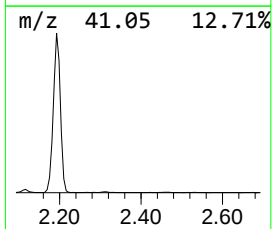
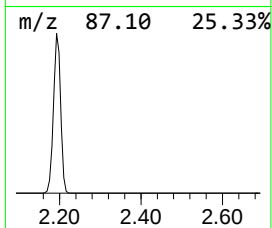
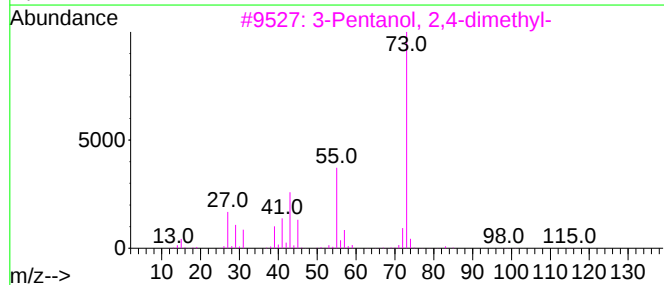
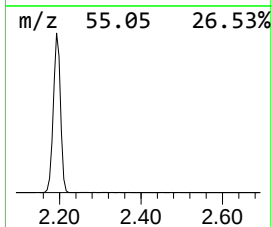
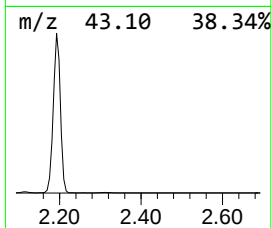
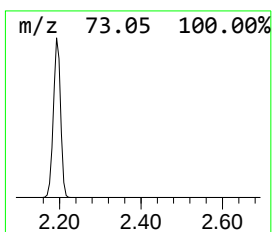
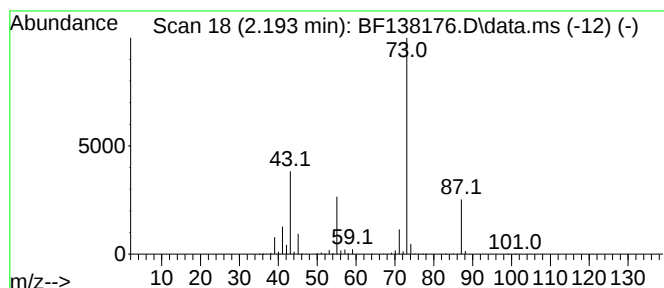
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	48.96 ng	5545830	1,4-Dichlorobenzene-d4	6.893

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	39
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25



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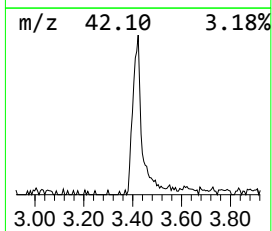
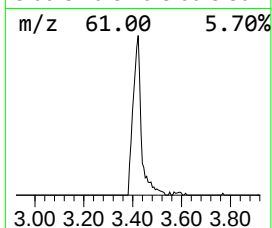
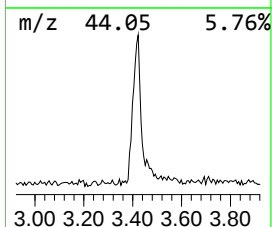
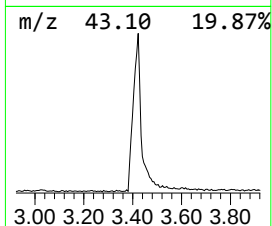
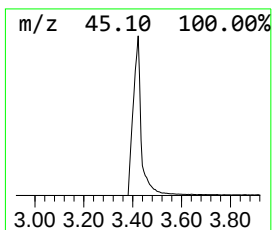
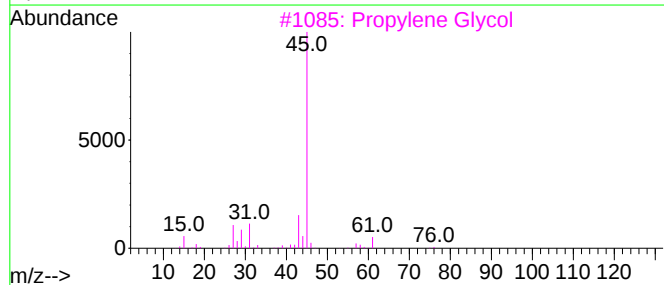
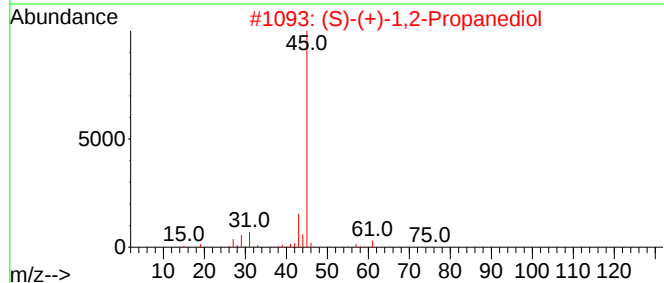
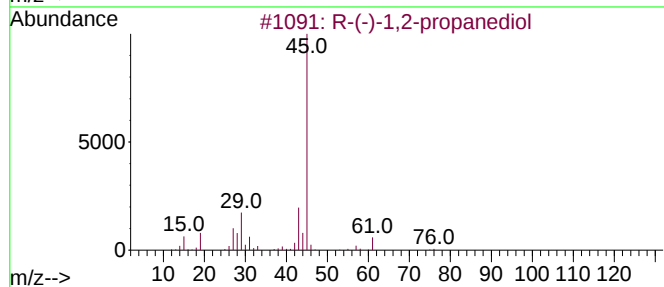
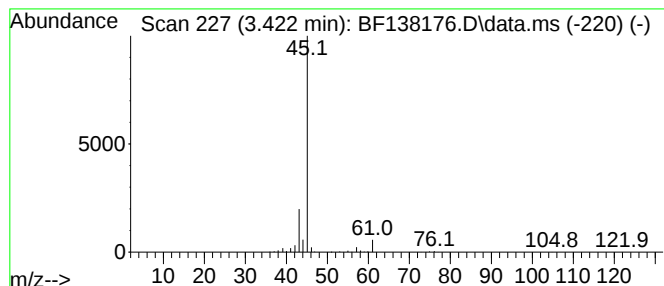
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Peak Number 2 R-(-)-1,2-propanediol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.422	7.00 ng	792349	1,4-Dichlorobenzene-d4	6.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	83
2	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	64
3	Propylene Glycol			76	C3H8O2	000057-55-6	64
4	Isopropyl Alcohol			60	C3H8O	000067-63-0	56
5	2-Pentanol			88	C5H12O	006032-29-7	9



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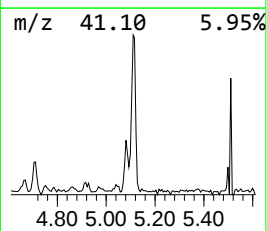
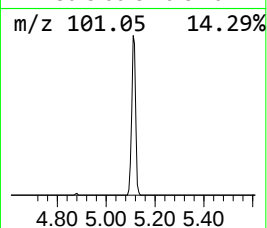
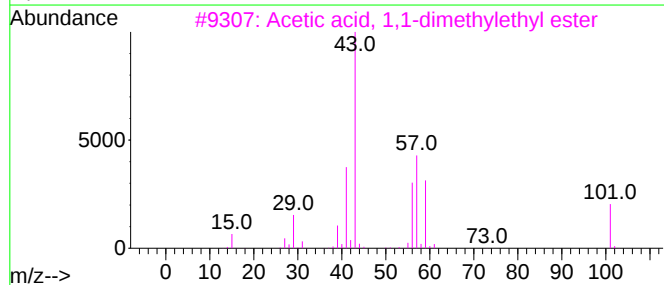
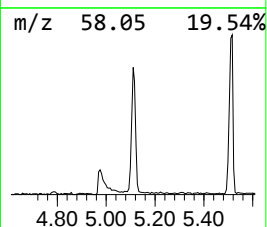
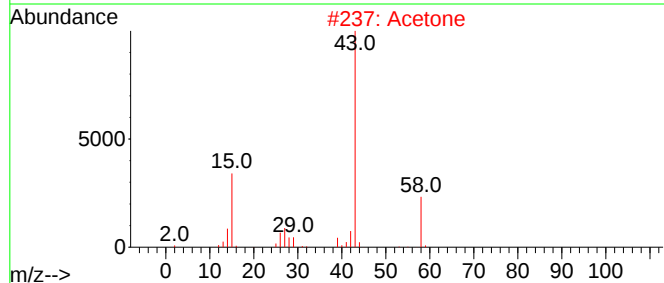
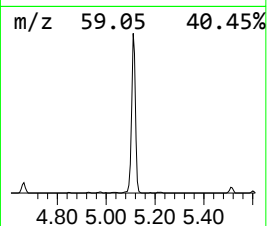
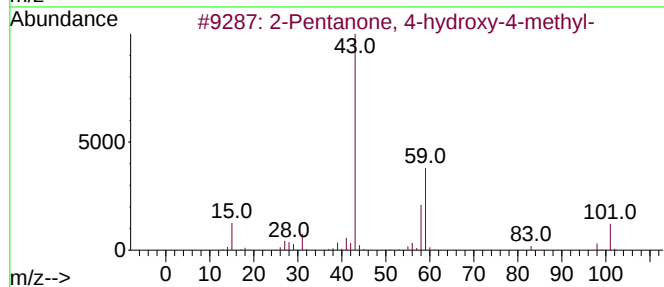
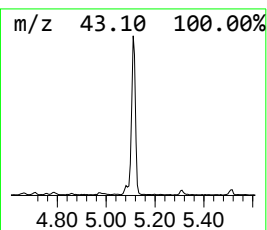
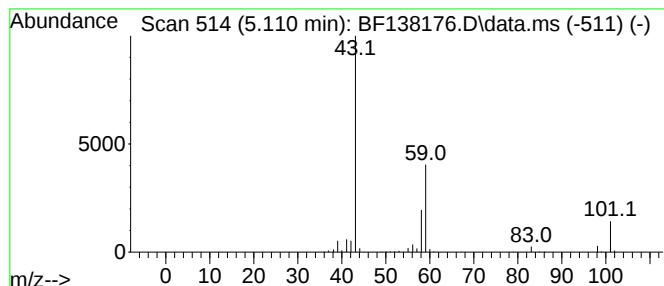
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TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	3.00 ng	340198	1,4-Dichlorobenzene-d4	6.893

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	83	
2	Acetone	58	C3H6O	000067-64-1	16	
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9	
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9	
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	7	



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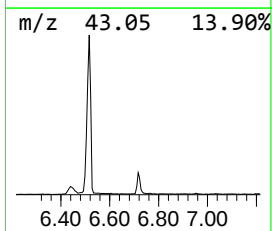
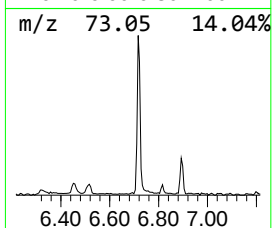
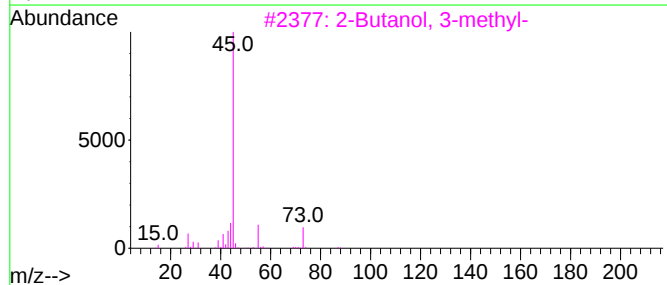
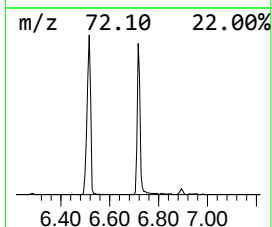
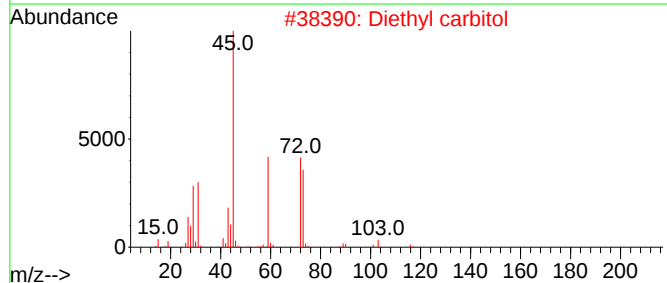
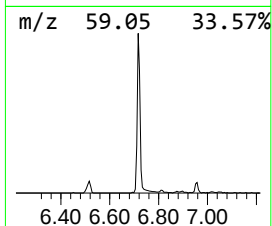
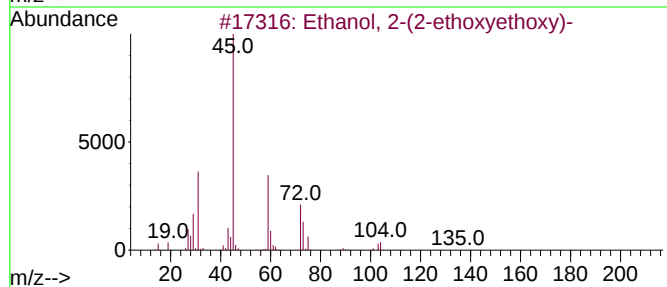
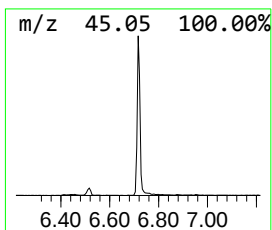
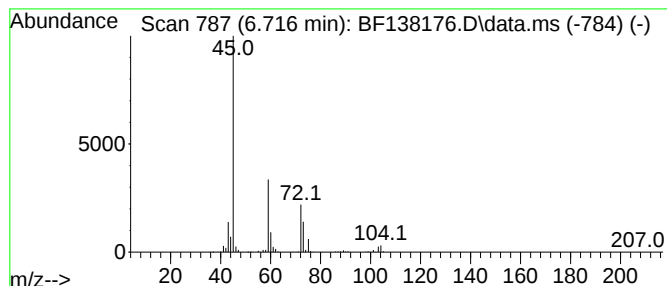
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.716	3.35 ng	379866	1,4-Dichlorobenzene-d4	6.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2			Diethyl carbitol	162	C8H18O3	000112-36-7	72
3			2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	47
4			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
5			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	39



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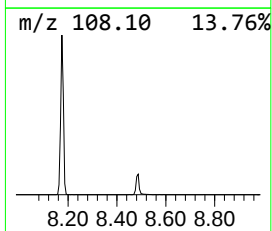
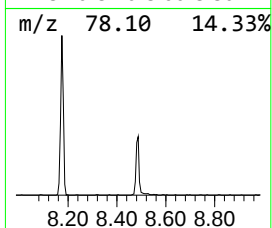
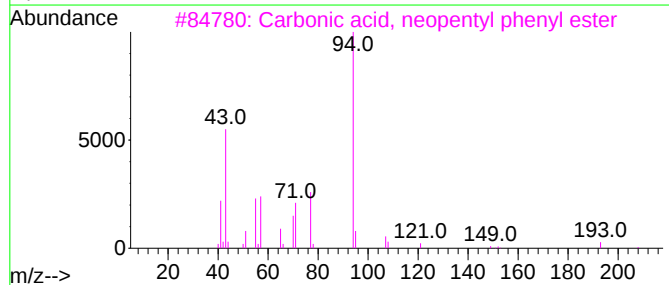
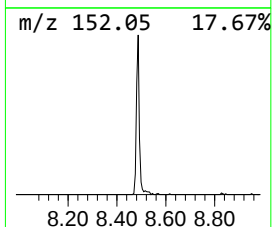
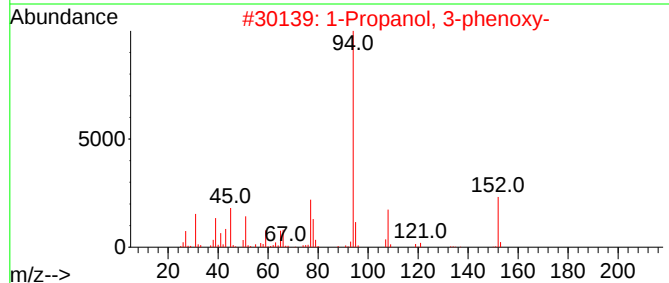
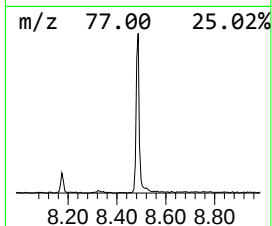
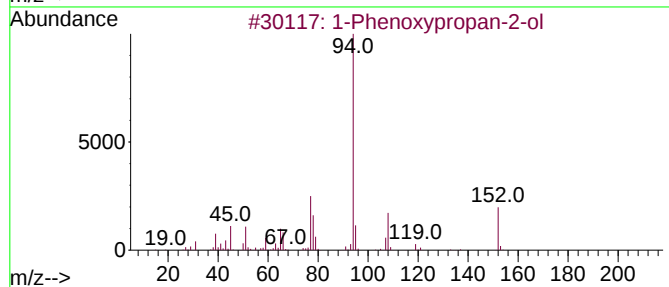
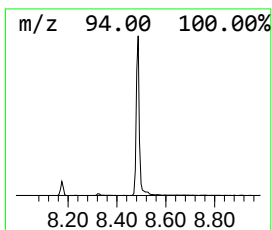
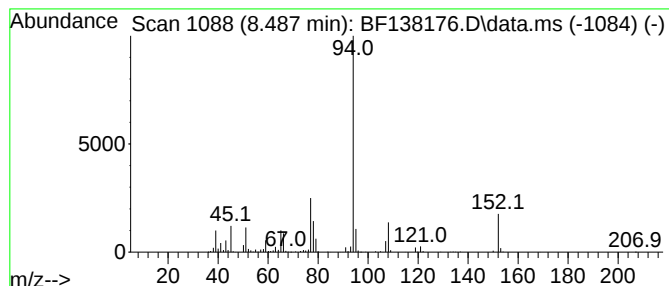
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Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.487	3.25 ng	485906	Naphthalene-d8	8.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	93
3			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64
4			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
5			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59



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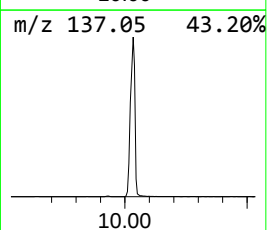
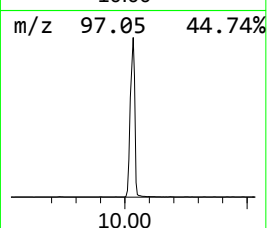
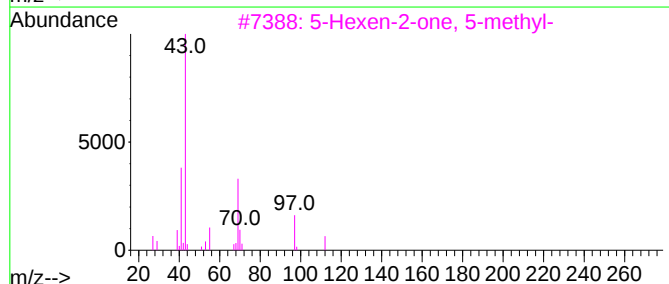
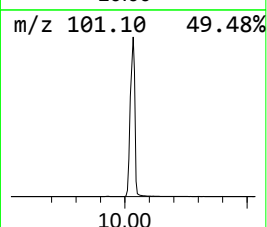
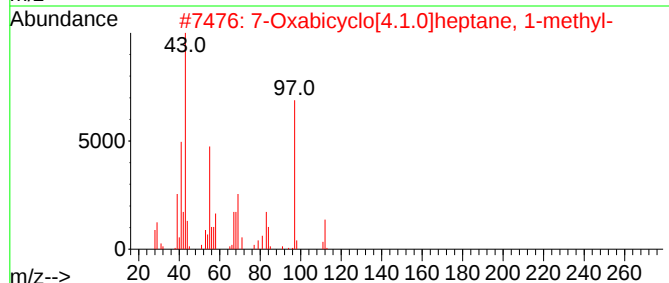
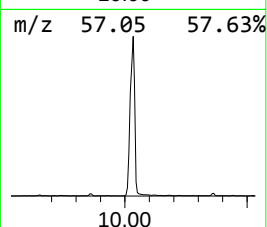
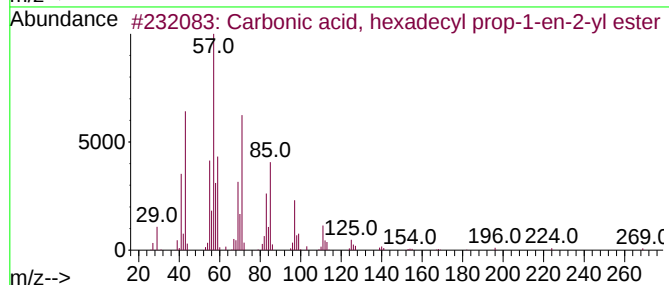
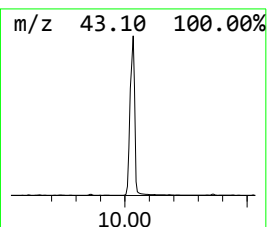
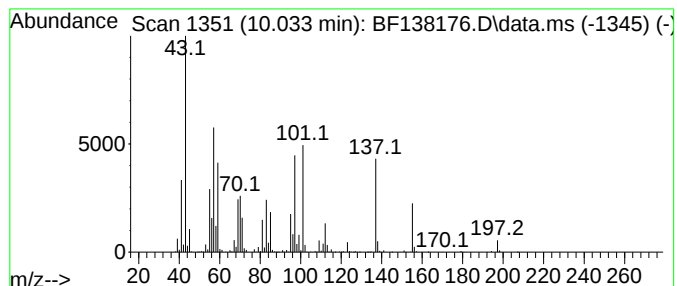
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown10.034 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.034	49.64 ng	8397630	Acenaphthene-d10	9.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	16
2			7-Oxabicyclo[4.1.0]heptane, 1-me...	112	C7H12O	001713-33-3	11
3			5-Hexen-2-one, 5-methyl-	112	C7H12O	003240-09-3	10
4			4,7-Dimethyl-5-decyne-4,7-diol	198	C12H22O2	000126-87-4	10
5			Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061024\
Data File : BF138176.D
Acq On : 10 Jun 2024 17:09
Operator : CG\JU
Sample : P2784-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

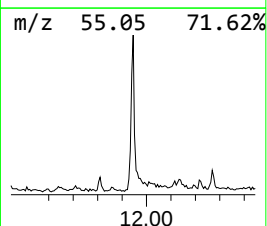
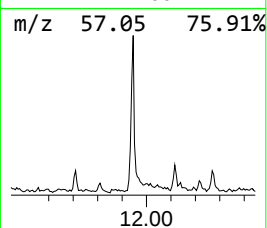
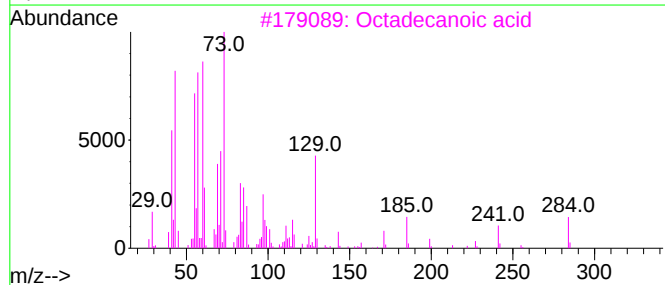
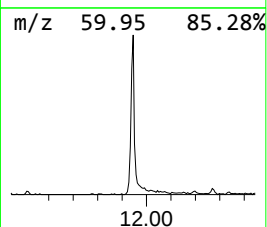
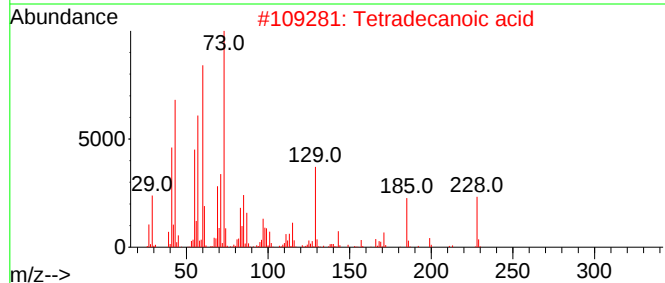
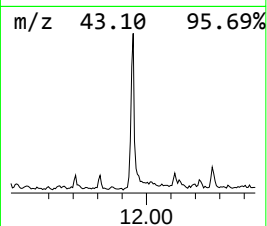
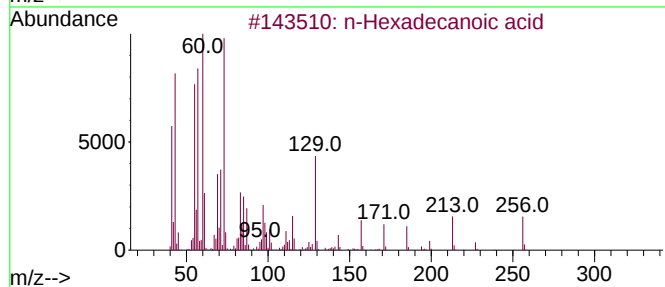
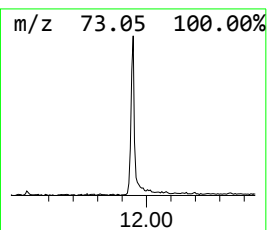
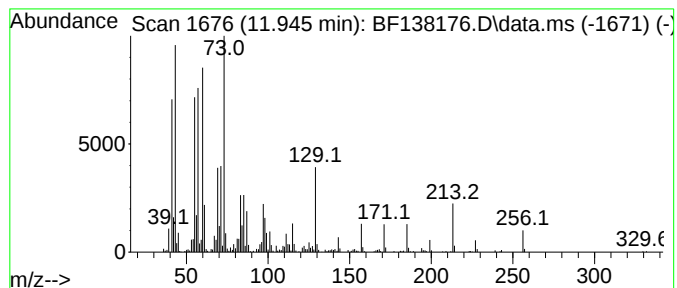
Instrument :
BNA_F
ClientSampleId :
WCS-TPD

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.945	3.43 ng	523382	Phenanthrene-d10		11.416	
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	94
3	Octadecanoic acid		284	C18H36O2	000057-11-4	90
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	90
5	Tridecanoic acid		214	C13H26O2	000638-53-9	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061024\
Data File : BF138176.D
Acq On : 10 Jun 2024 17:09
Operator : CG\JU
Sample : P2784-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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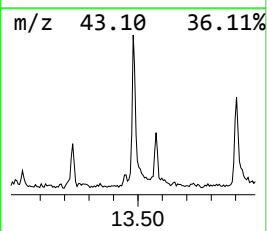
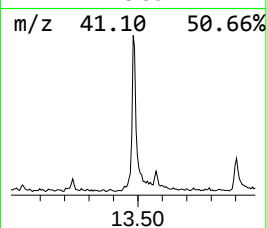
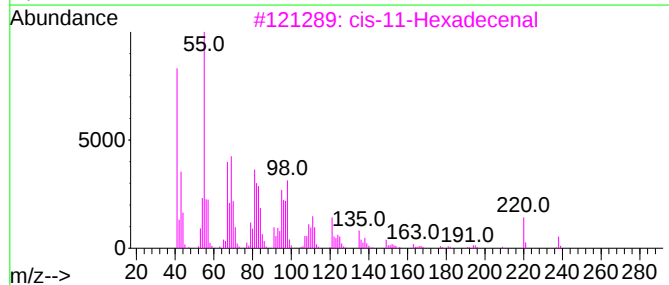
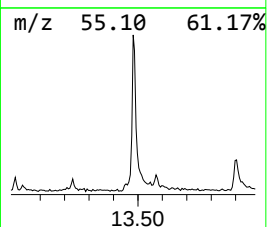
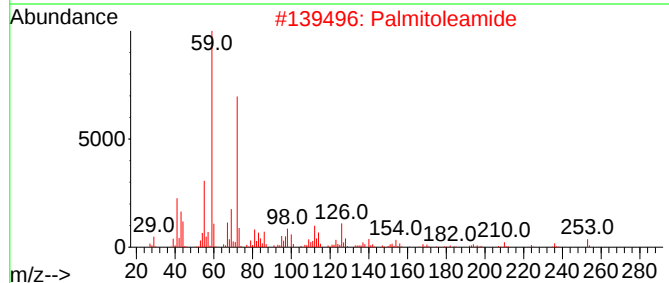
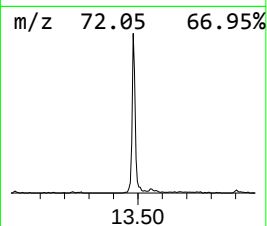
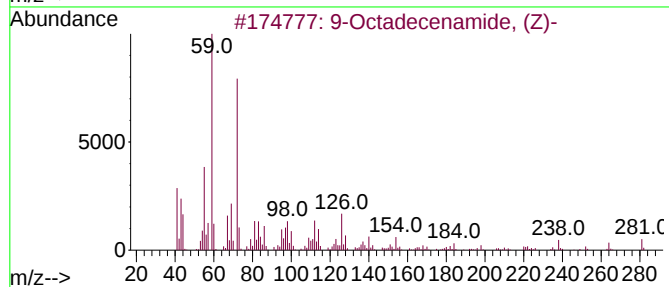
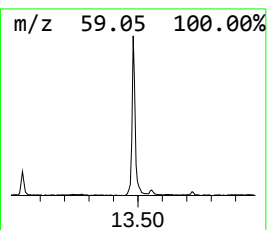
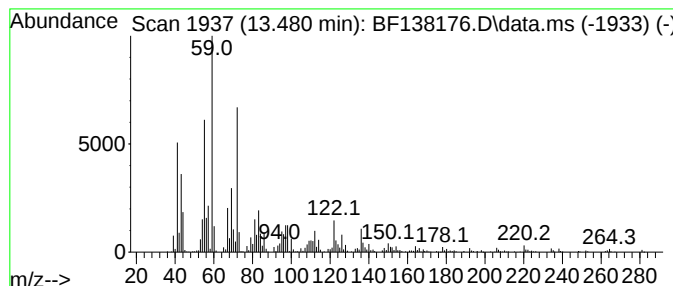
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.480	6.62 ng	678544	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	96
2			Palmitoleamide	253	C16H31NO	106010-22-4	70
3			cis-11-Hexadecenal	238	C16H30O	053939-28-9	41
4			E-9-Hexadecenal	238	C16H30O	1000130-90-3	41
5			2,7-Dioxatricyclo[4.4.0.0(3,8)]d...	155	C8H13NO2	040076-28-6	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061024\
Data File : BF138176.D
Acq On : 10 Jun 2024 17:09
Operator : CG\JU
Sample : P2784-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

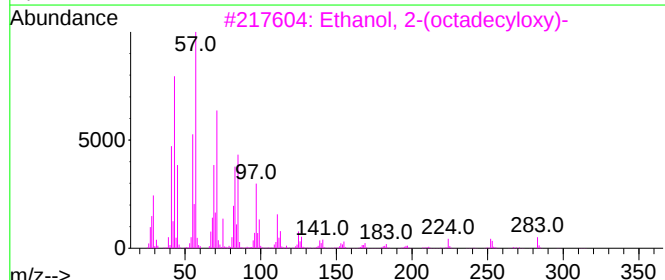
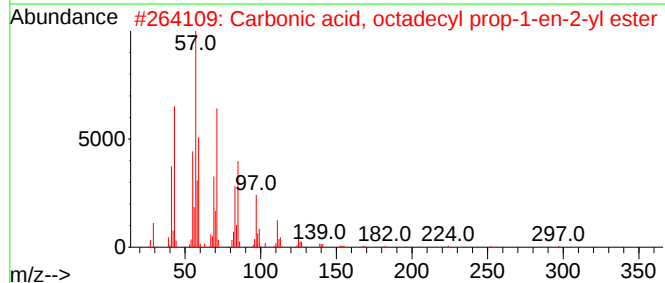
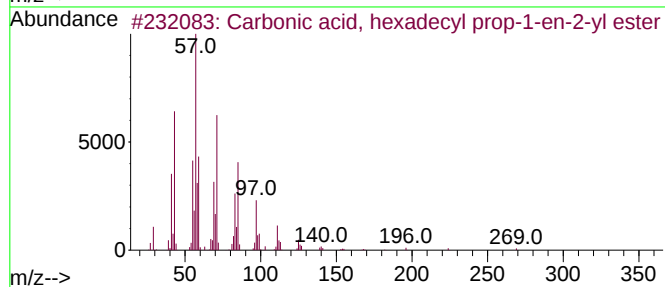
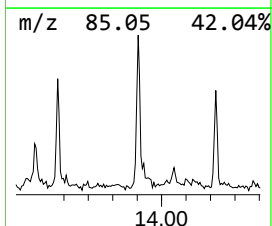
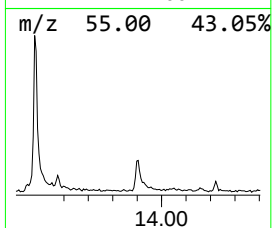
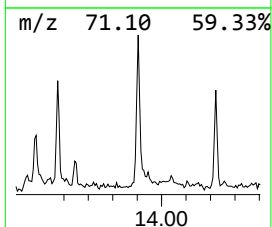
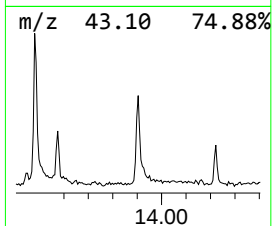
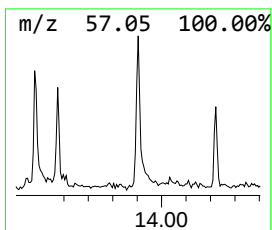
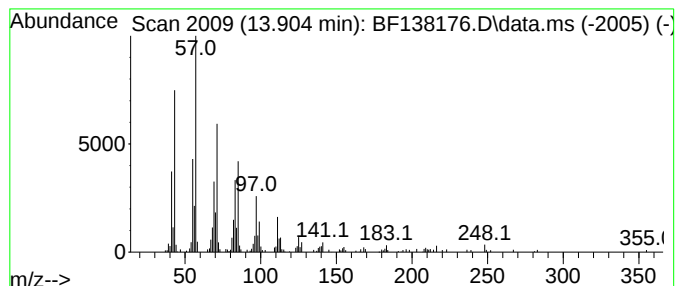
Instrument :
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ClientSampleId :
WCS-TPD

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Carbonic acid, hexadecyl pr... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.904	2.06 ng	211571	Chrysene-d12	14.051	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	91
2	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	91
3	Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	91
4	Carbonic acid, decyl hexadecyl e...	426	C27H54O3	1000383-16-5	90
5	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061024\
Data File : BF138176.D
Acq On : 10 Jun 2024 17:09
Operator : CG\JU
Sample : P2784-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WCS-TPD

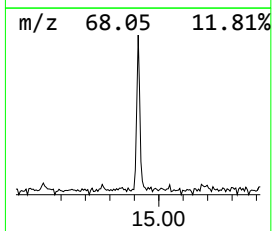
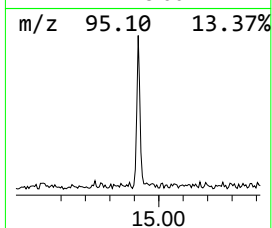
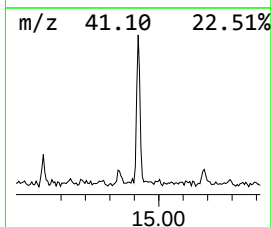
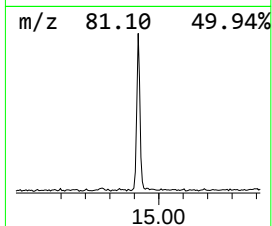
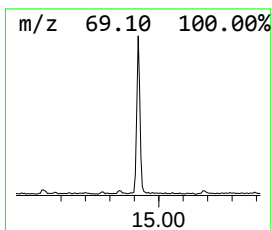
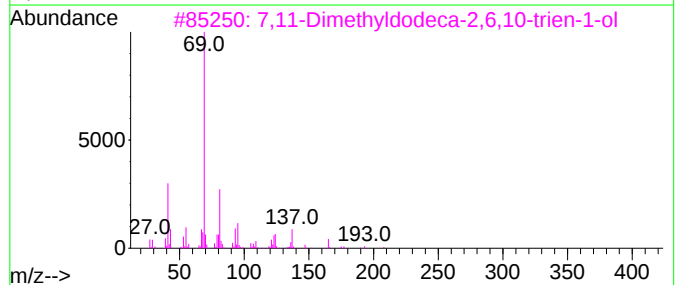
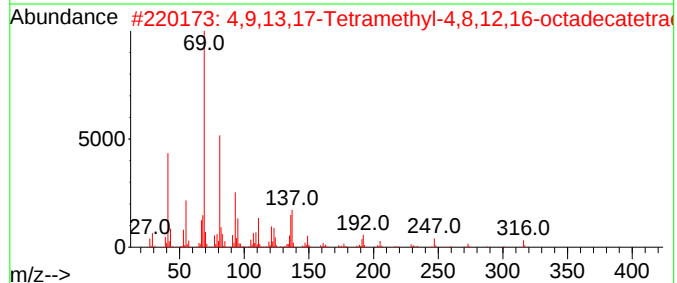
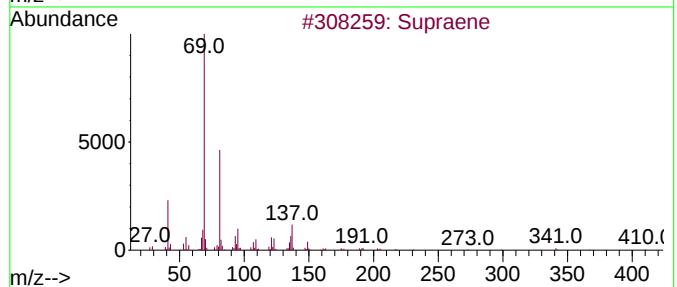
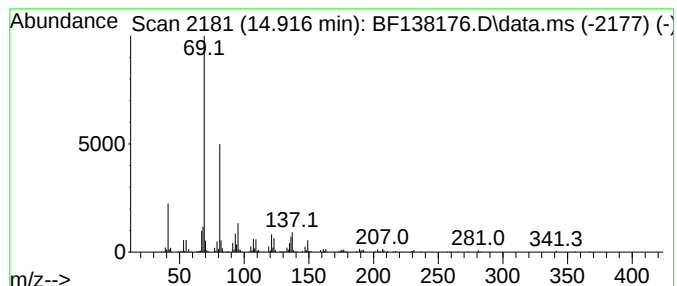
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Supraene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.916	2.43 ng	244133	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
3			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	83
4			.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
5			1-(Phenylthio)-3,7,11-trimethyl-...	314	C21H30S	028413-57-2	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061024\
Data File : BF138176.D
Acq On : 10 Jun 2024 17:09
Operator : CG\JU
Sample : P2784-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WCS-TPD

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.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	49.0	ng	5545830	1	6.893	2265260	20.0
R-(-)-1,2-propa...	3.422	7.0	ng	792349	1	6.893	2265260	20.0
2-Pentanone, 4-...	5.110	3.0	ng	340198	1	6.893	2265260	20.0
Ethanol, 2-(2-e...	6.716	3.4	ng	379866	1	6.893	2265260	20.0
1-Phenoxypropan...	8.487	3.3	ng	485906	2	8.175	2993360	20.0
unknown10.034	10.034	49.6	ng	8397630	3	9.928	3383380	20.0
n-Hexadecanoic ...	11.945	3.4	ng	523382	4	11.416	3052460	20.0
9-Octadecenamid...	13.480	6.6	ng	678544	5	14.051	2049170	20.0
Carbonic acid, ...	13.904	2.1	ng	211571	5	14.051	2049170	20.0
Supraene	14.916	2.4	ng	244133	6	15.527	2006760	20.0