

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060624\
 Data File : BF138145.D
 Acq On : 06 Jun 2024 21:14
 Operator : CG\JU
 Sample : P2718-03
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-4

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: BF138145.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	17	24	28	rVB	9761605	13975336	100.00%	19.835%
2	3.057	158	165	173	rVB	777942	1239588	8.87%	1.759%
3	5.122	513	516	522	rVB	255566	269498	1.93%	0.382%
4	5.522	579	584	587	rBV	4336193	3717178	26.60%	5.276%
5	6.522	749	754	757	rBV	2582147	2363323	16.91%	3.354%
6	6.728	786	789	794	rBV	168820	158635	1.14%	0.225%
7	6.904	815	819	822	rBV	2957881	2257224	16.15%	3.204%
8	7.469	909	915	918	rBV	5650003	5255083	37.60%	7.458%
9	8.086	1016	1020	1028	rBV	282756	261258	1.87%	0.371%
10	8.186	1033	1037	1040	rBV	3904355	3027533	21.66%	4.297%
11	8.492	1086	1089	1099	rVB	667470	538132	3.85%	0.764%
12	9.263	1215	1220	1223	rBV	11844098	10582192	75.72%	15.019%
13	9.939	1331	1335	1338	rBV	4557974	3598423	25.75%	5.107%
14	10.727	1464	1469	1472	rBV	7335352	6540944	46.80%	9.283%
15	11.427	1584	1588	1591	rBV	4166382	3509676	25.11%	4.981%
16	11.951	1673	1677	1687	rBV2	441790	485091	3.47%	0.688%
17	13.016	1853	1858	1861	rBV	10098709	9117097	65.24%	12.940%
18	13.910	2006	2010	2019	rBV2	394197	467194	3.34%	0.663%
19	14.063	2032	2036	2051	rBV	1867323	1641087	11.74%	2.329%
20	15.545	2281	2288	2304	rBV	1106937	1454079	10.40%	2.064%

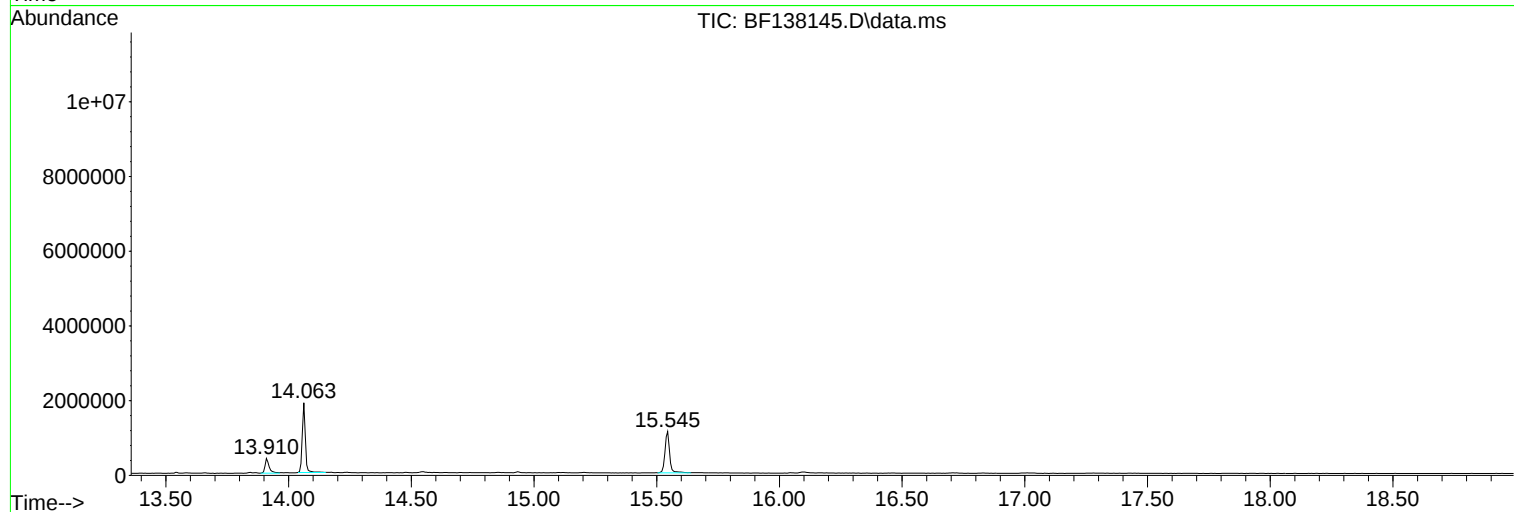
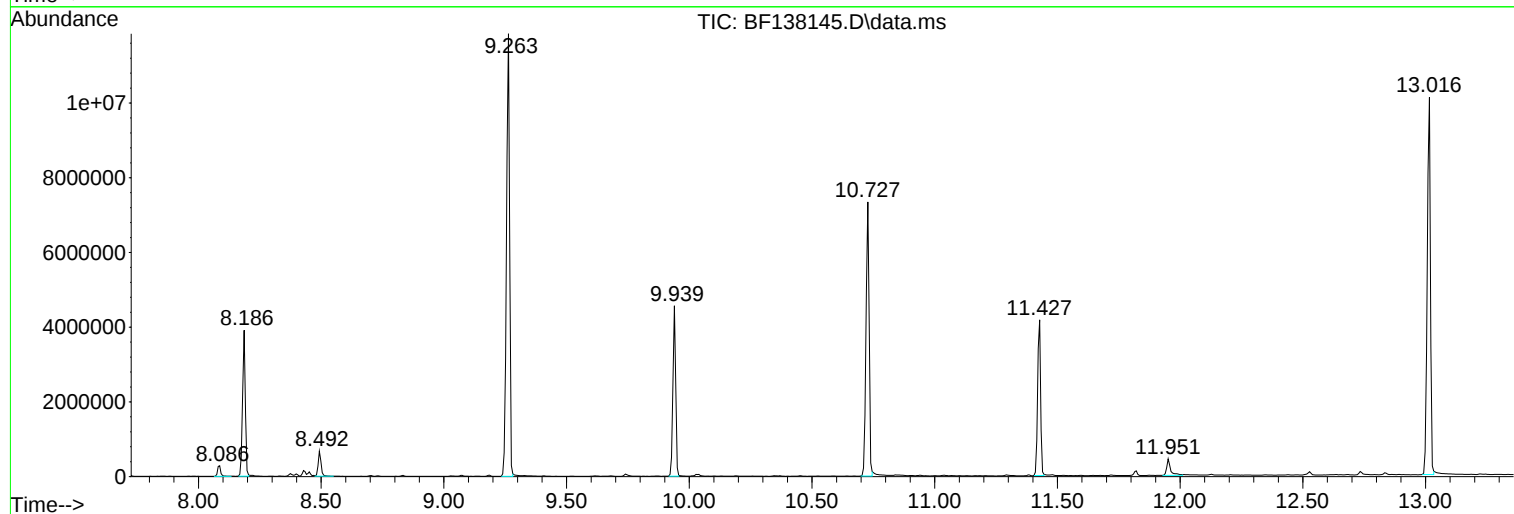
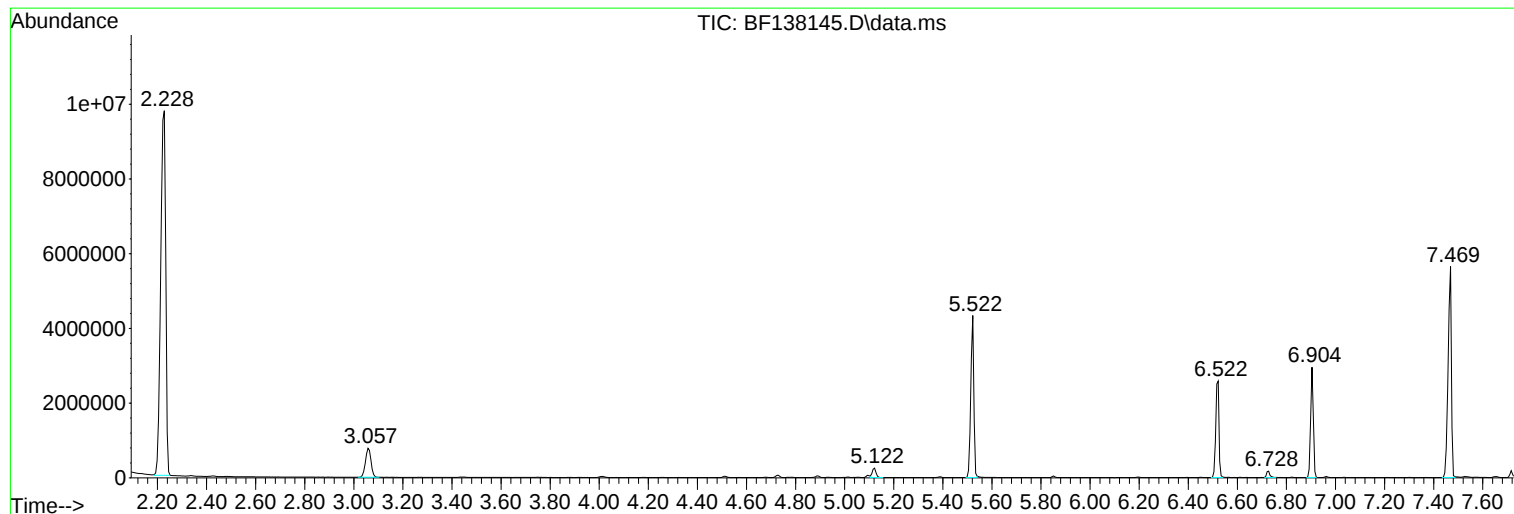
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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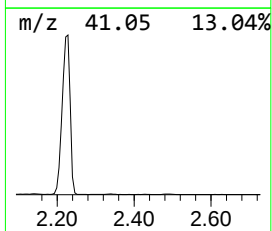
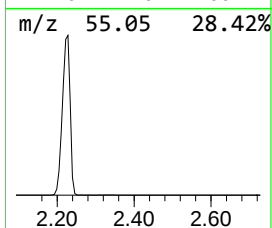
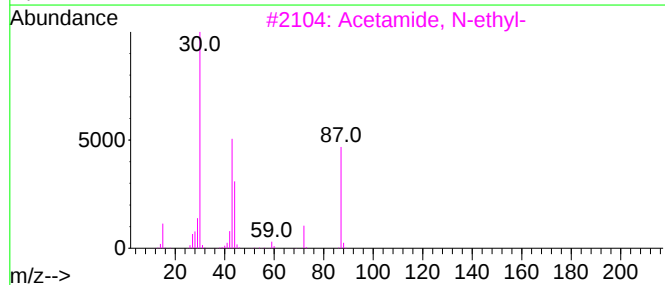
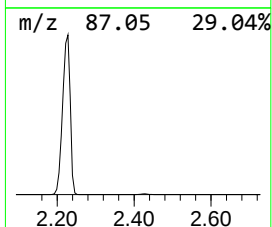
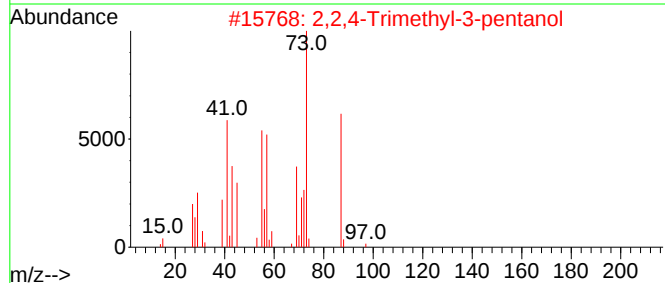
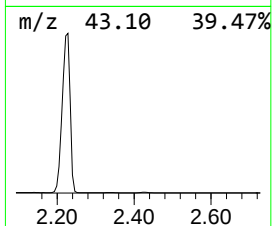
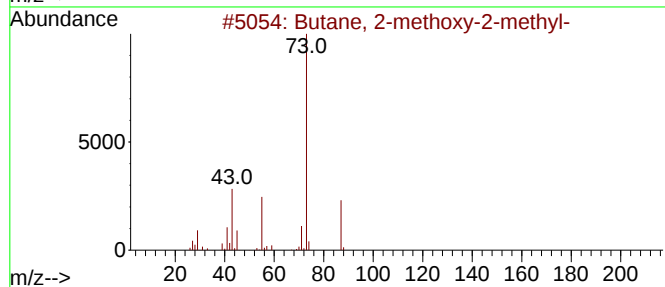
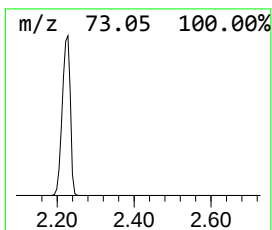
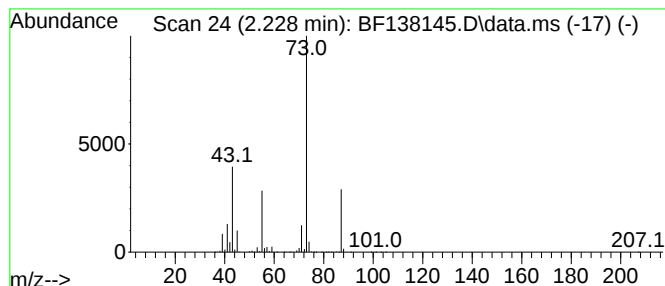
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.228	123.83 ng	13975300	1,4-Dichlorobenzene-d4	6.904

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			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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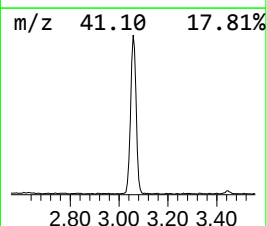
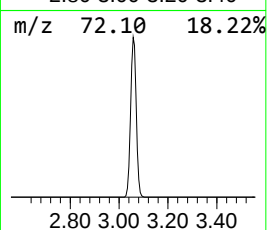
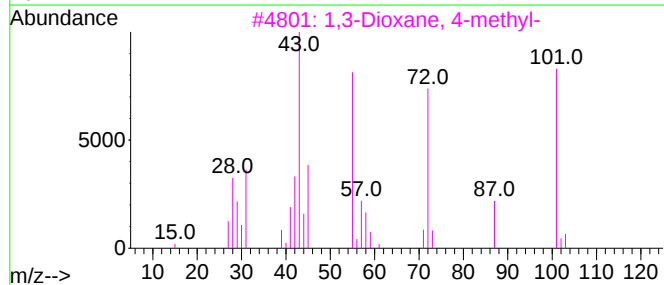
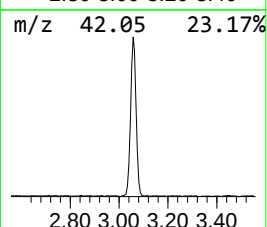
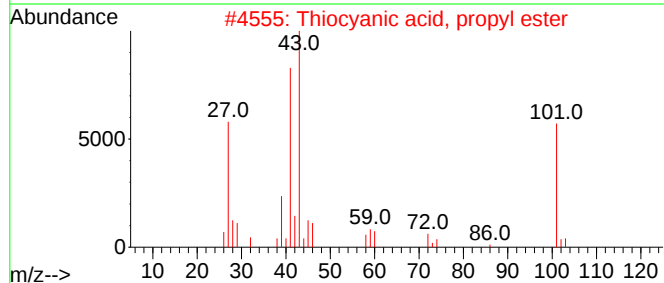
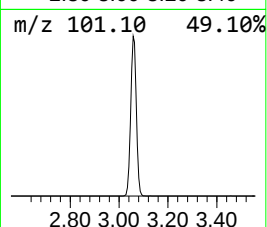
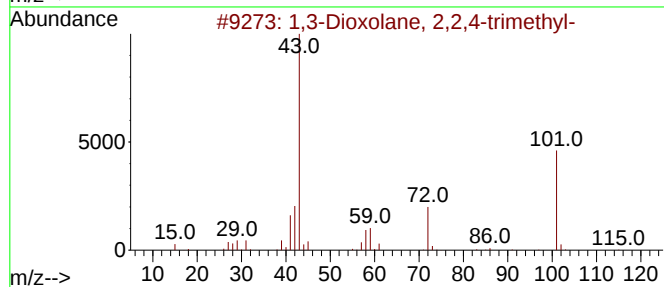
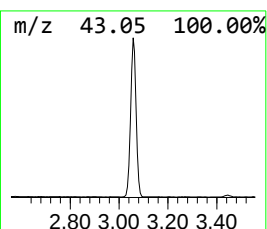
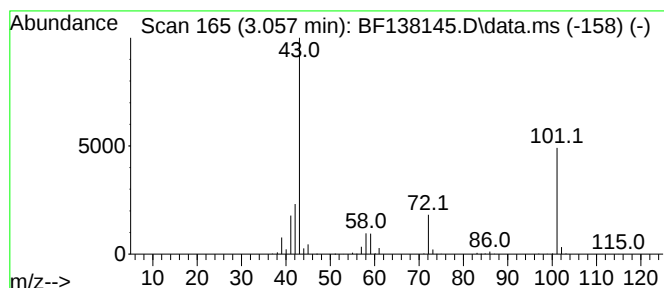
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
3.057	10.98 ng	1239590	1,4-Dichlorobenzene-d4	6.904	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	90
2	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	59
3	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	50
4	Allyl acetate	100	C5H8O2	000591-87-7	9
5	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9



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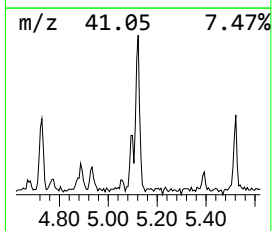
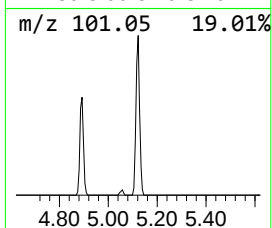
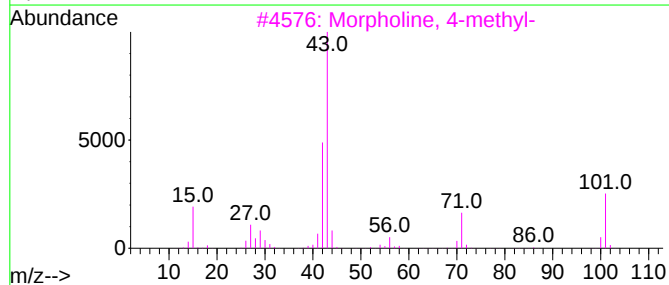
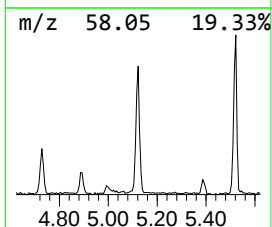
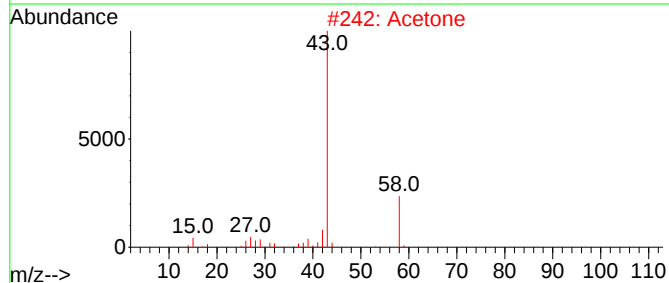
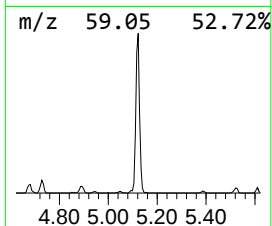
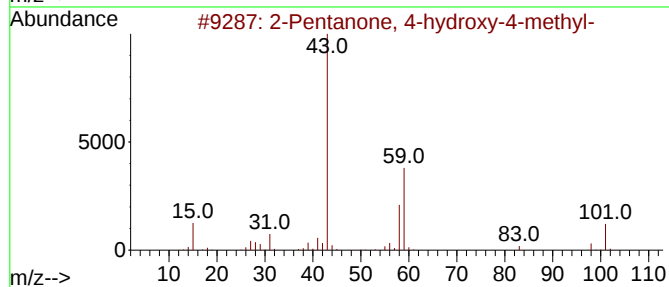
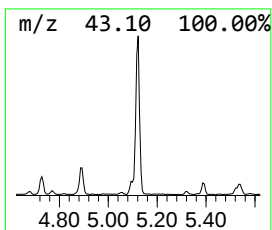
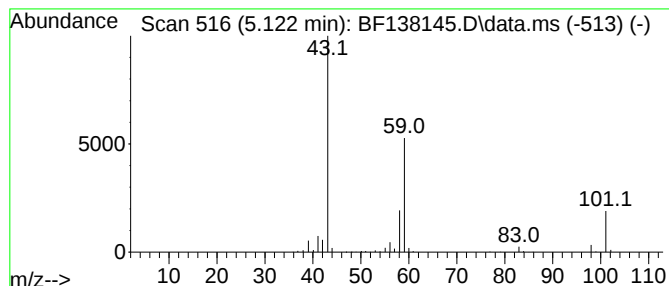
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	2.39 ng	269498	1,4-Dichlorobenzene-d4	6.904

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetone	58	C3H6O	000067-64-1	16
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Amylene hydrate	88	C5H12O	000075-85-4	9
5		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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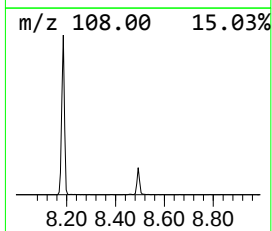
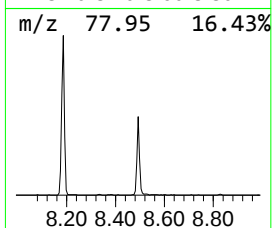
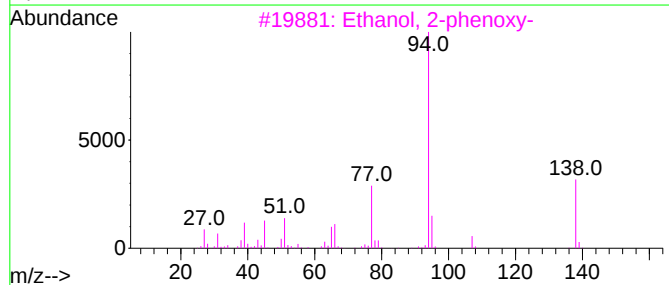
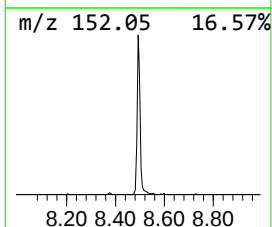
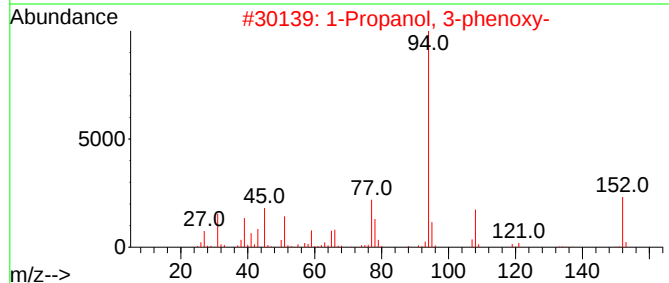
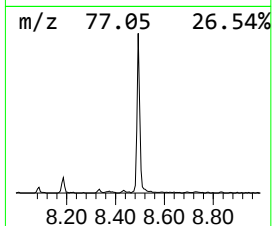
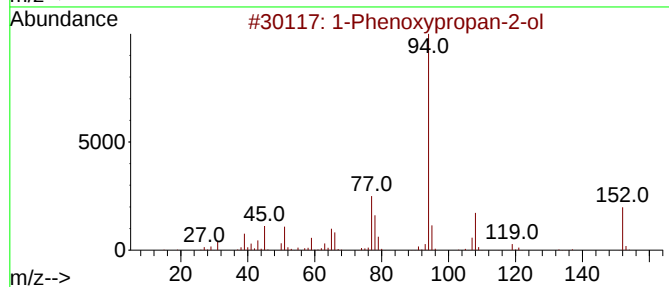
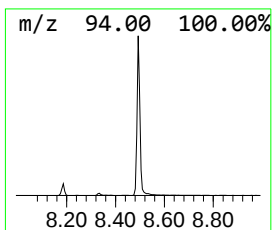
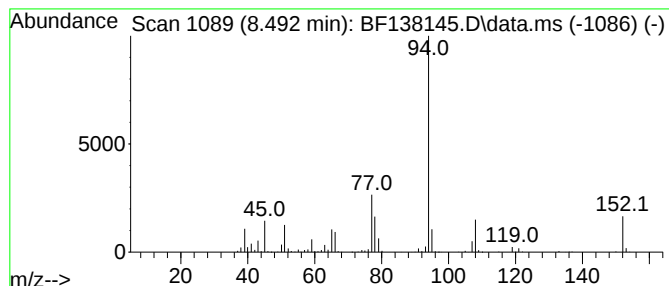
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TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.492	3.55 ng	538132	Naphthalene-d8	8.186

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	87
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
5			tert-Butyl phenyl carbonate	194	C11H14O3	006627-89-0	53



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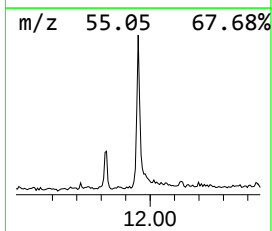
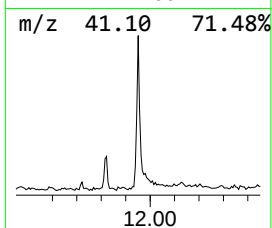
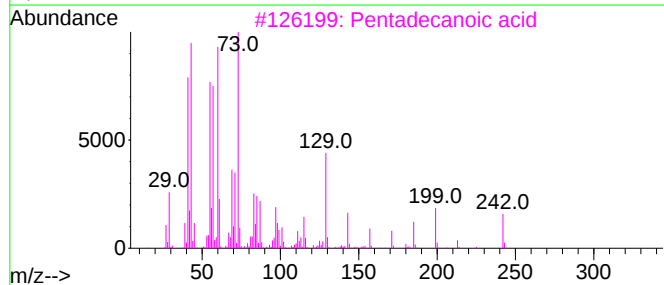
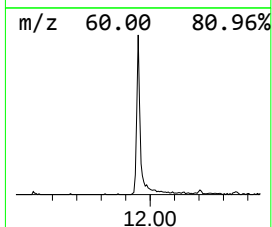
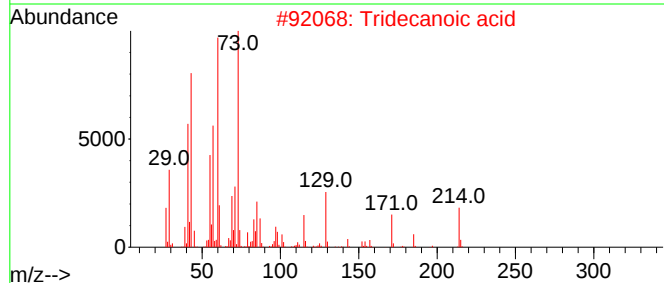
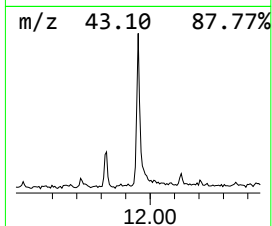
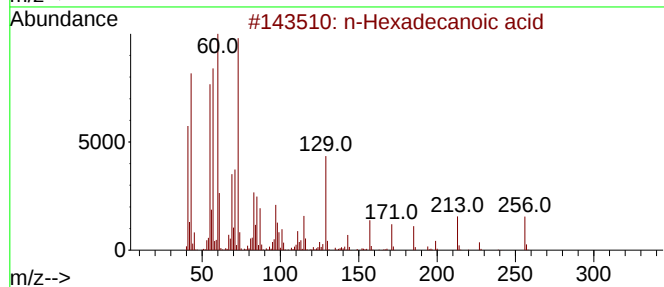
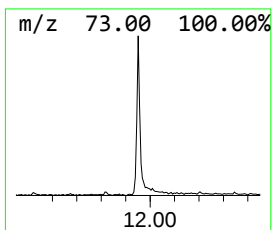
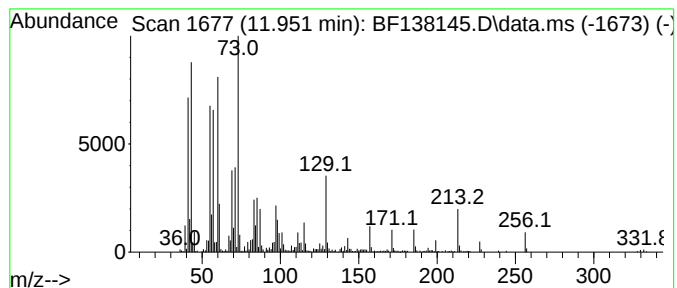
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.951	2.76 ng	485091	Phenanthrene-d10		11.427	
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	91
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	87
4	Octadecanoic acid		284	C18H36O2	000057-11-4	87
5	Tetradecanoic acid		228	C14H28O2	000544-63-8	83



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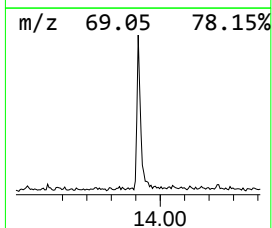
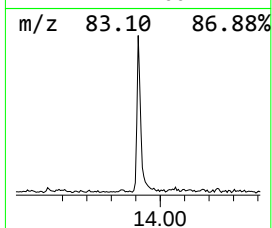
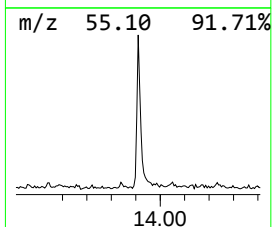
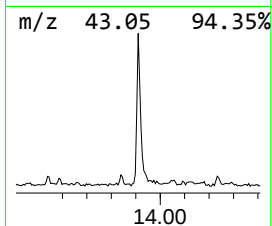
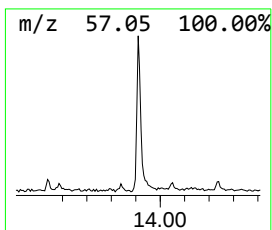
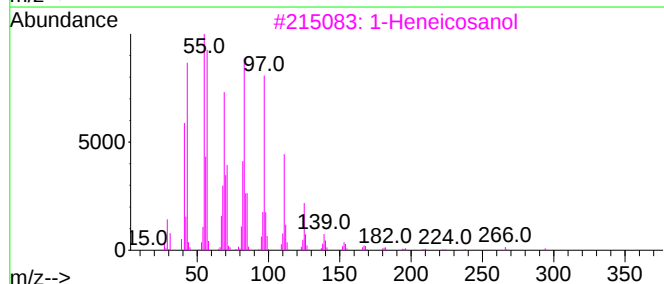
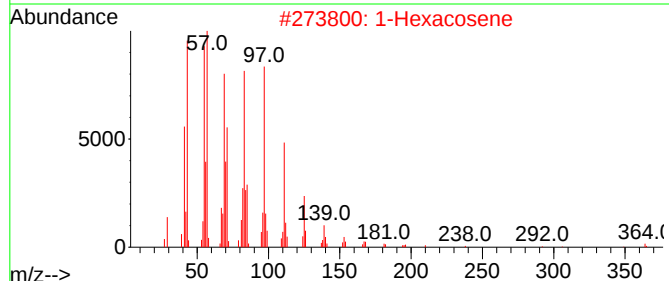
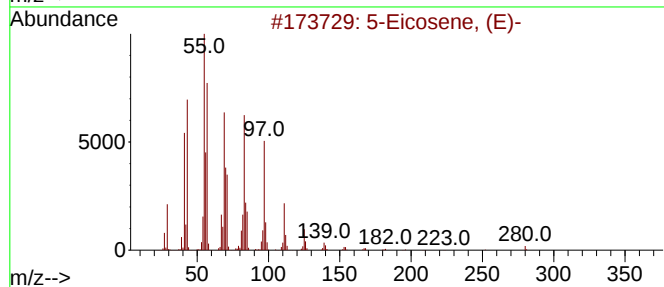
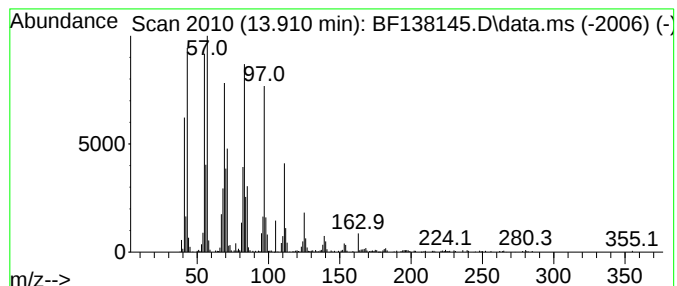
Instrument :
BNA_F
ClientSampleId :
MW-4

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 6 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.910	5.69 ng	467194	Chrysene-d12	14.063	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	1-Hexacosene	364	C26H52	018835-33-1	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
5	Behenic alcohol	326	C22H46O	000661-19-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060624\
Data File : BF138145.D
Acq On : 06 Jun 2024 21:14
Operator : CG\JU
Sample : P2718-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.228	123.8	ng	13975300	1	6.904	2257220	20.0
1,3-Dioxolane, ...	3.057	11.0	ng	1239590	1	6.904	2257220	20.0
2-Pentanone, 4-...	5.122	2.4	ng	269498	1	6.904	2257220	20.0
1-Phenoxypropan...	8.492	3.5	ng	538132	2	8.186	3027530	20.0
n-Hexadecanoic ...	11.951	2.8	ng	485091	4	11.427	3509680	20.0
5-Eicosene, (E)-	13.910	5.7	ng	467194	5	14.063	1641090	20.0