

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
 Data File : BF139101.D
 Acq On : 21 Aug 2024 14:51
 Operator : RC/JU
 Sample : P3357-05
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-857-J-SO-4-4.5-072024

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-BF082024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139101.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	10	17	24	rBV	993450	1552475	72.04%	8.852%
2	3.404	215	223	232	rBV	66839	157623	7.31%	0.899%
3	5.110	505	513	521	rVB	82033	120001	5.57%	0.684%
4	5.510	575	581	586	rBV	1397481	1839881	85.37%	10.491%
5	6.516	745	752	757	rBV	1373634	1906349	88.45%	10.870%
6	6.716	779	786	792	rBV	60174	74928	3.48%	0.427%
7	6.898	811	817	822	rVB	463075	586502	27.21%	3.344%
8	7.457	905	912	917	rBV	890676	1183305	54.91%	6.747%
9	7.710	950	955	959	rVB	21358	24735	1.15%	0.141%
10	8.175	1029	1034	1039	rBV	601217	755185	35.04%	4.306%
11	8.487	1082	1087	1092	rBV	141213	174823	8.11%	0.997%
12	9.251	1211	1217	1222	rBV	1724289	2155165	100.00%	12.288%
13	9.933	1327	1333	1338	rBV	665231	841438	39.04%	4.798%
14	10.028	1343	1349	1355	rBV	602420	902606	41.88%	5.146%
15	10.716	1461	1466	1477	rBV	1002804	1267834	58.83%	7.229%
16	11.416	1580	1585	1590	rVB	603949	729162	33.83%	4.158%
17	11.816	1649	1653	1657	rVB	19805	23294	1.08%	0.133%
18	11.945	1669	1675	1685	rBV2	47055	75827	3.52%	0.432%
19	12.522	1767	1773	1780	rVB2	19085	29501	1.37%	0.168%
20	12.874	1822	1833	1843	rBV	80987	156909	7.28%	0.895%
21	13.004	1849	1855	1860	rVB	1127608	1389513	64.47%	7.923%
22	13.904	2002	2008	2016	rBV2	109999	171178	7.94%	0.976%
23	14.051	2028	2033	2041	rVB	352637	450597	20.91%	2.569%
24	14.539	2110	2116	2122	rBV	74285	110582	5.13%	0.631%
25	15.198	2223	2228	2238	rBV2	35826	87538	4.06%	0.499%
26	15.280	2238	2242	2252	rVB	19421	32856	1.52%	0.187%
27	15.533	2279	2285	2291	rBV	349991	525815	24.40%	2.998%
28	16.039	2366	2371	2374	rBV	16795	28899	1.34%	0.165%
29	16.086	2374	2379	2387	rVV	47798	98625	4.58%	0.562%
30	16.162	2387	2392	2400	rVB	14851	33409	1.55%	0.190%
31	17.262	2572	2579	2589	rBV9	7741	23481	1.09%	0.134%
32	17.639	2637	2643	2652	rBV6	12133	28246	1.31%	0.161%

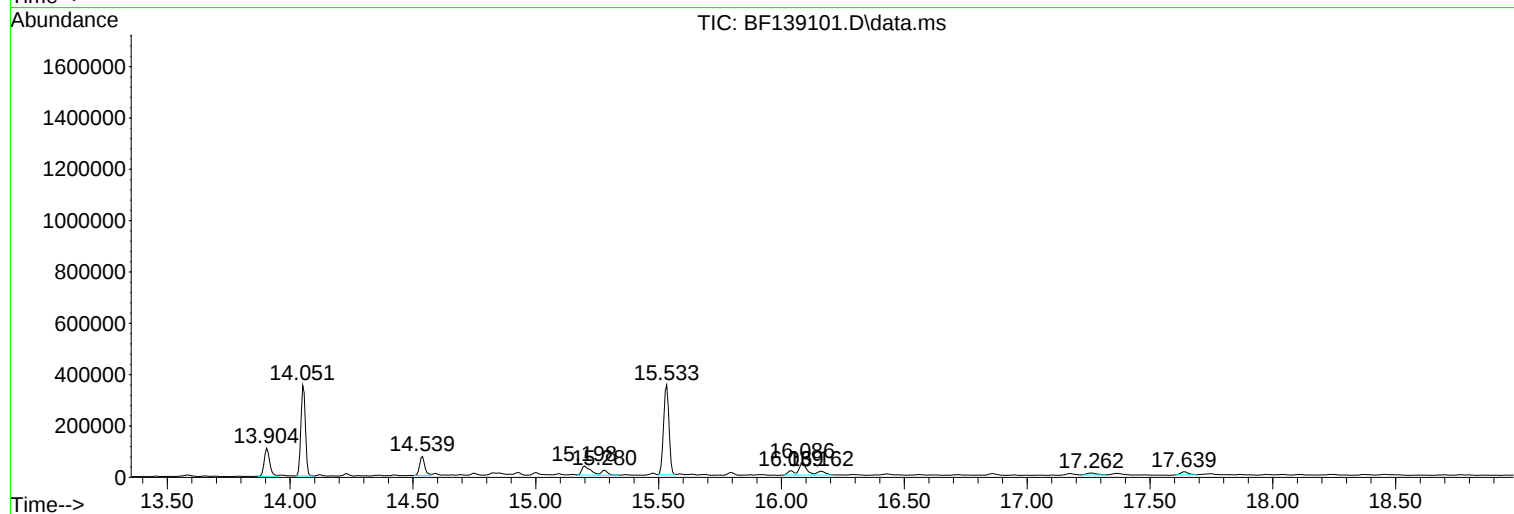
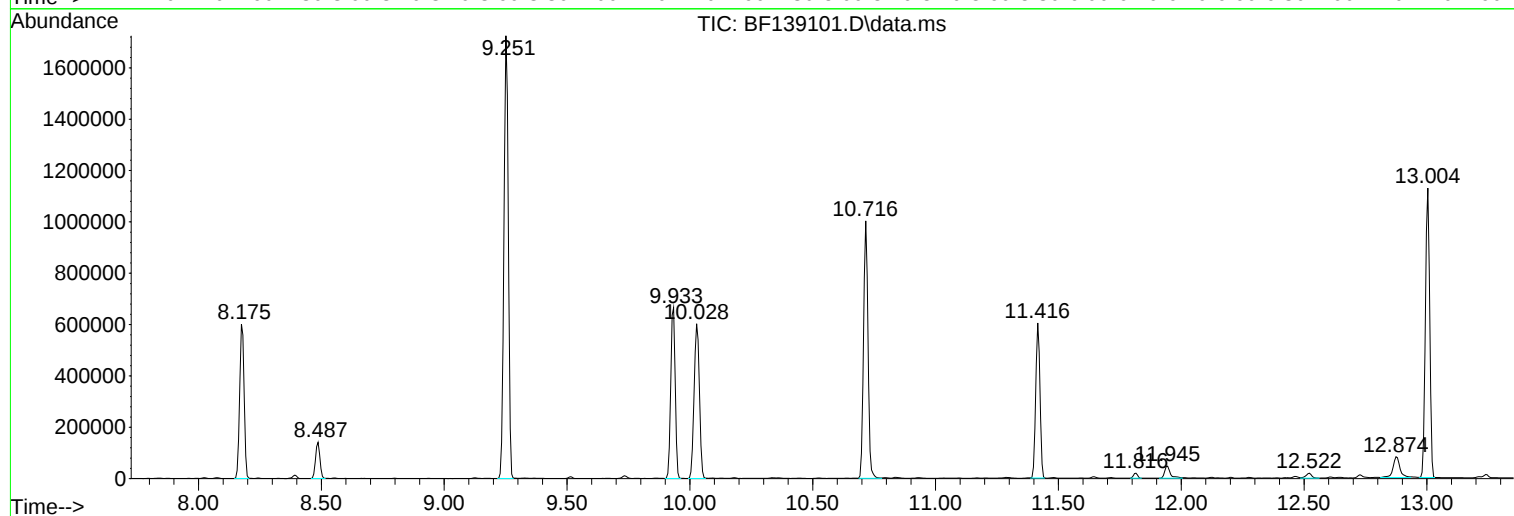
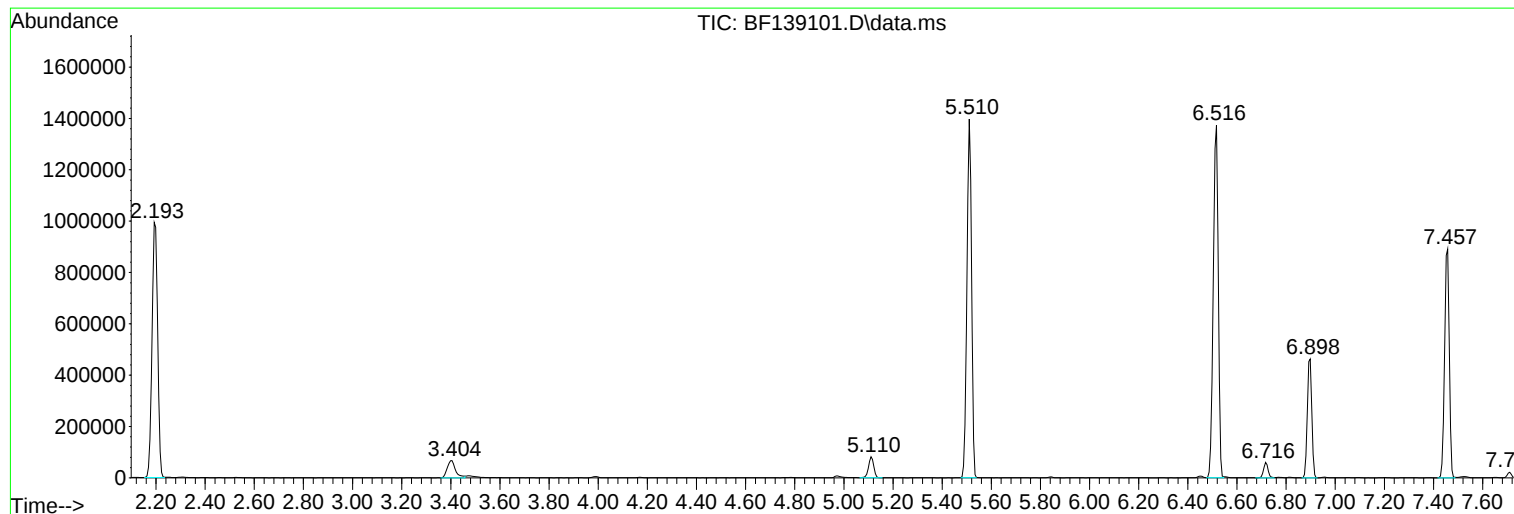
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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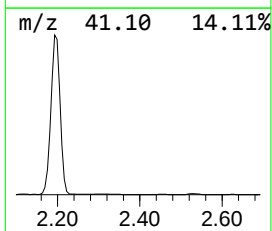
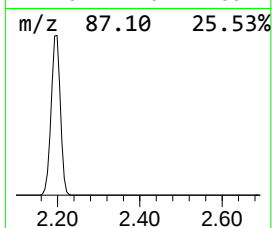
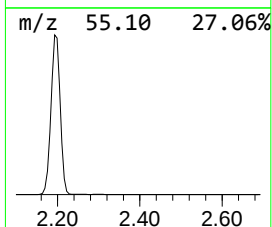
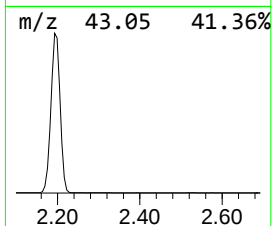
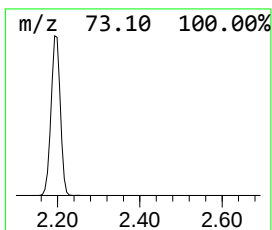
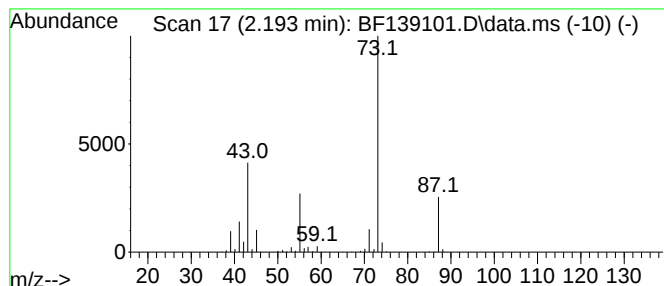
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.193	52.94 ng	1552480	1,4-Dichlorobenzene-d4	6.898

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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	10



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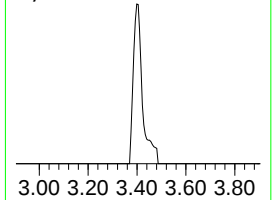
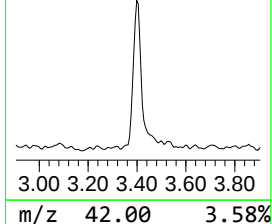
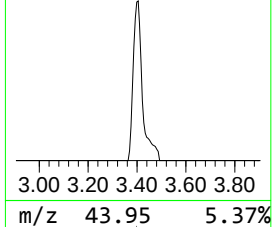
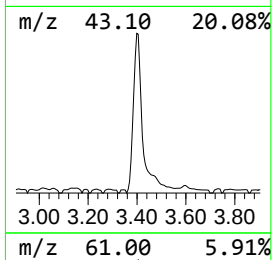
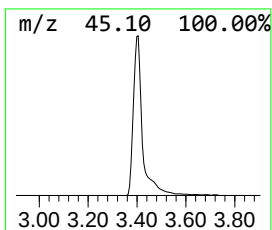
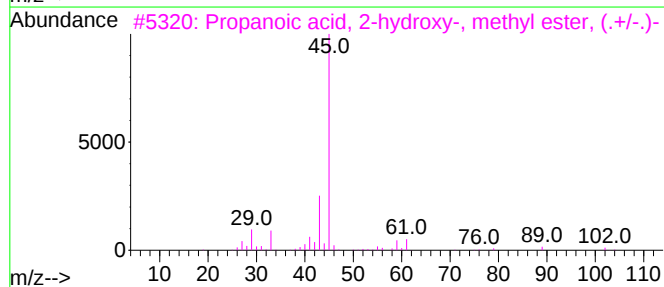
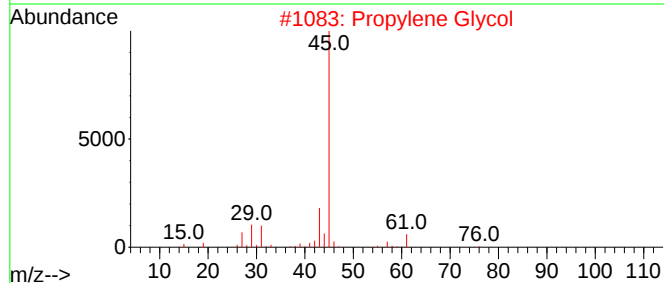
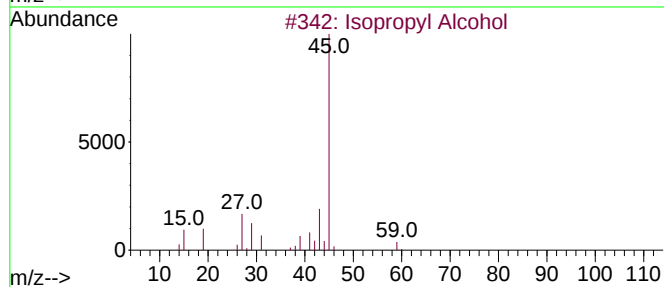
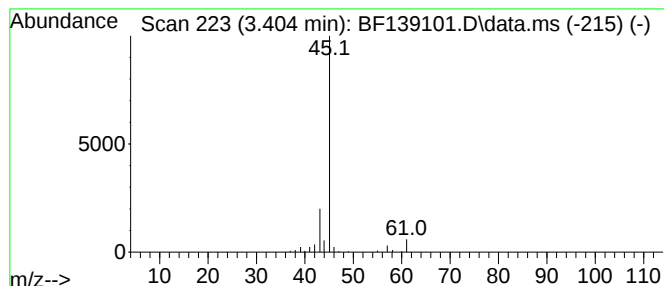
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Isopropyl Alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.404	5.38 ng	157623	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
2			Propylene Glycol	76	C3H8O2	000057-55-6	43
3			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
4			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
5			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9



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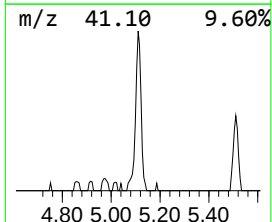
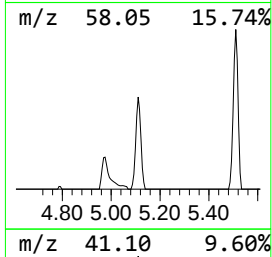
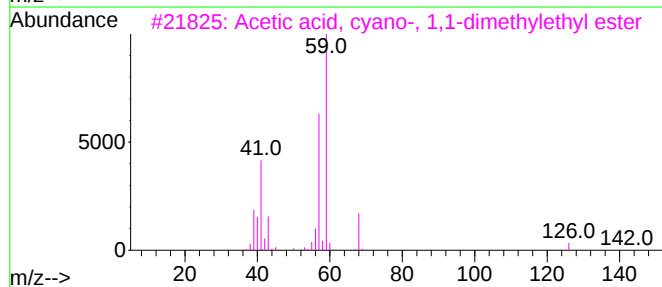
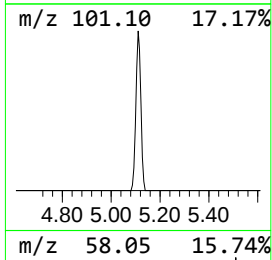
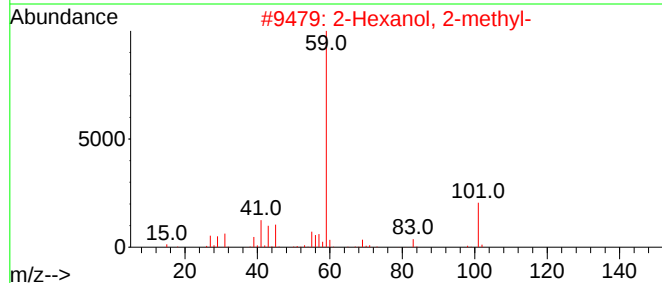
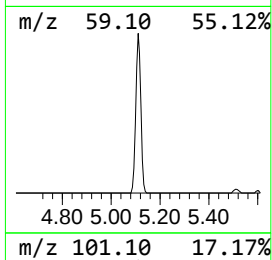
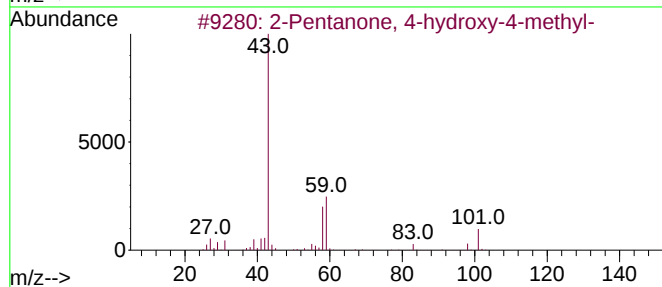
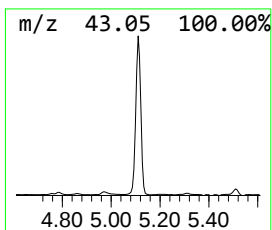
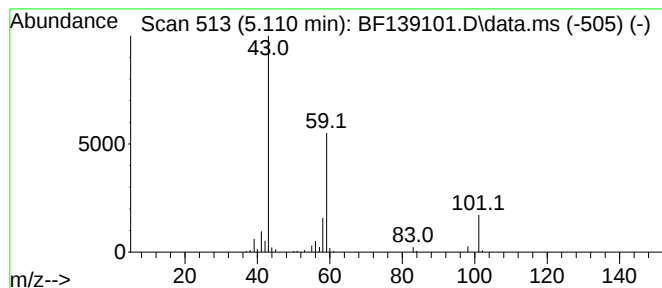
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	4.09 ng	120001	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9



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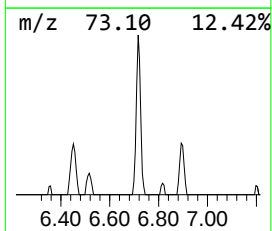
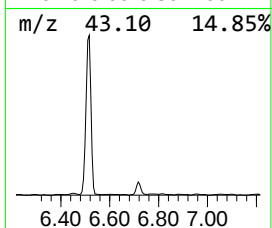
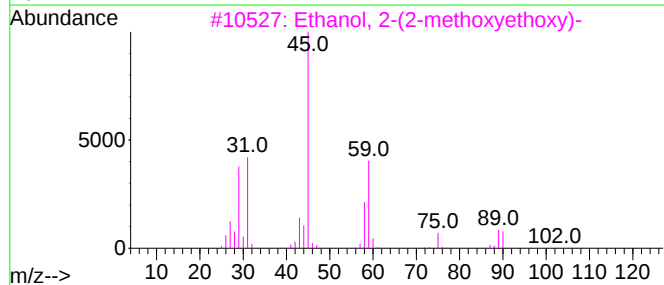
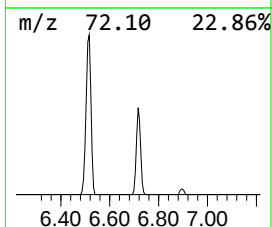
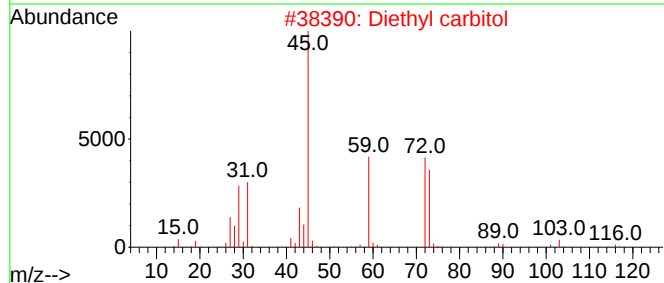
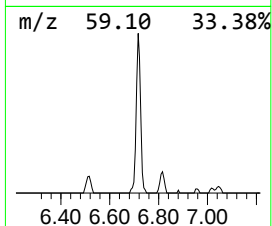
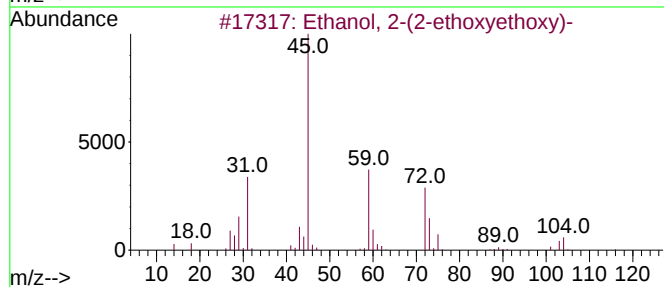
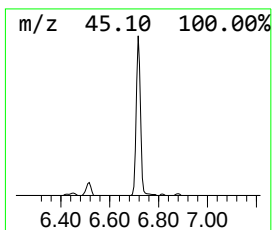
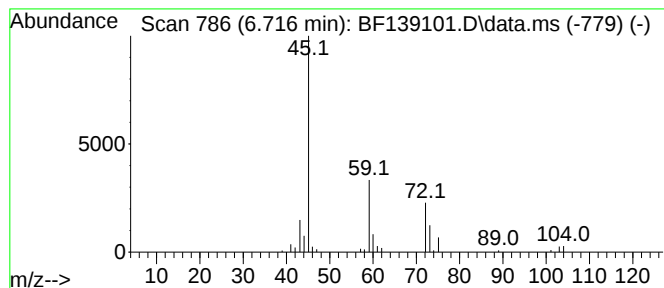
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.716	2.56 ng	74928	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			Diethyl carbitol	162	C8H18O3	000112-36-7	78
3			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	45
4			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	40
5			Ethanol, 2,2'-oxybis-	106	C4H10O3	000111-46-6	38



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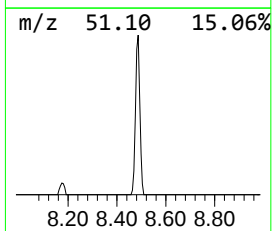
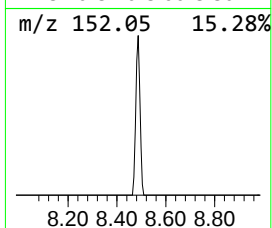
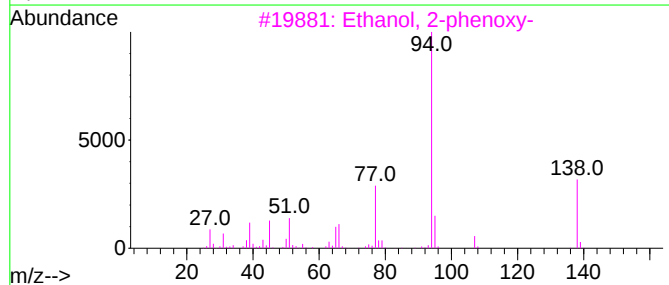
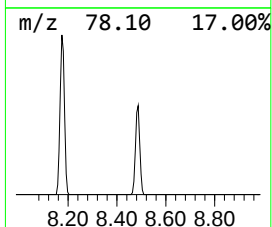
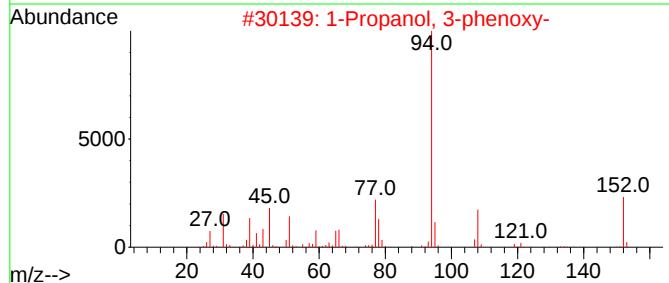
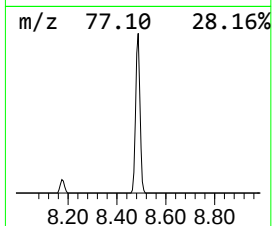
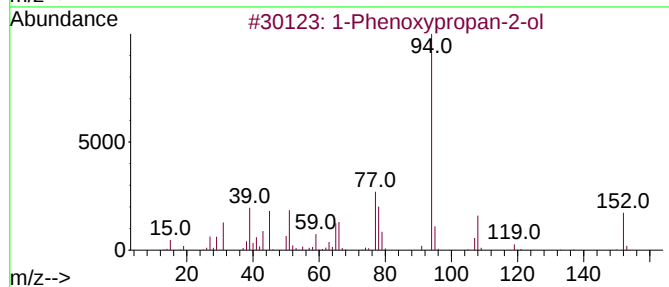
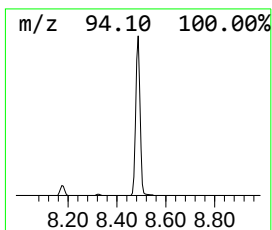
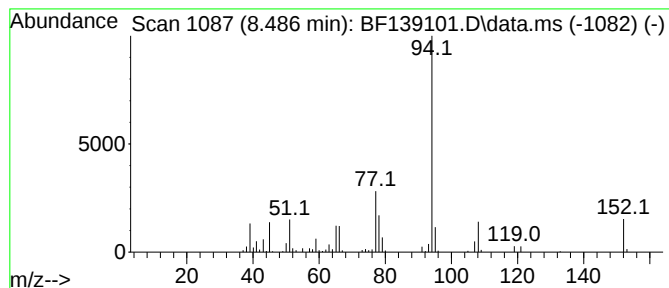
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Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.486	4.63 ng	174823	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	87
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
5			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59



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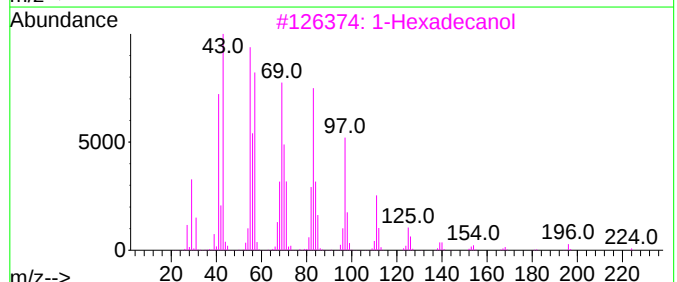
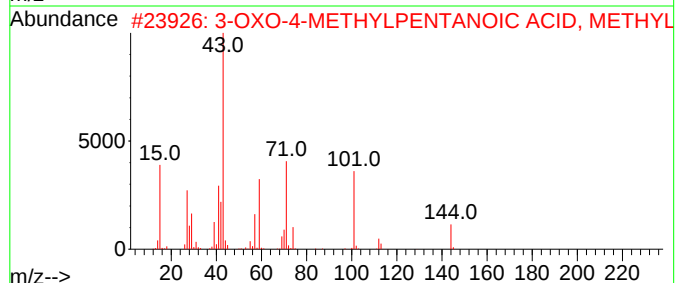
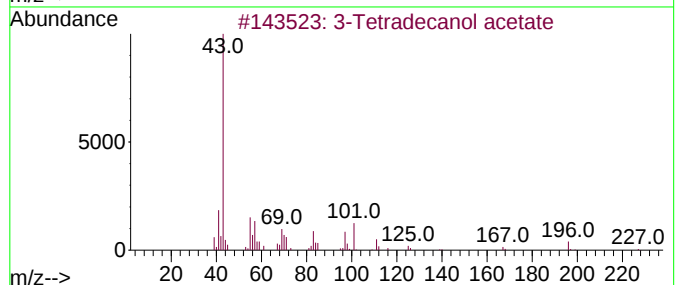
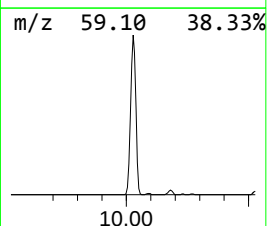
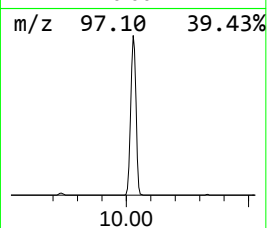
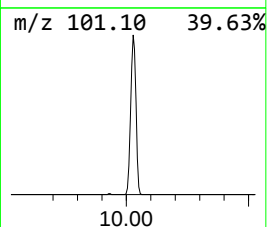
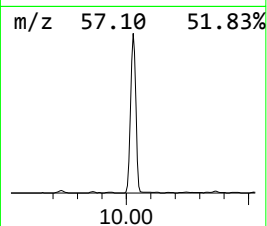
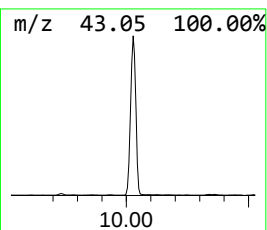
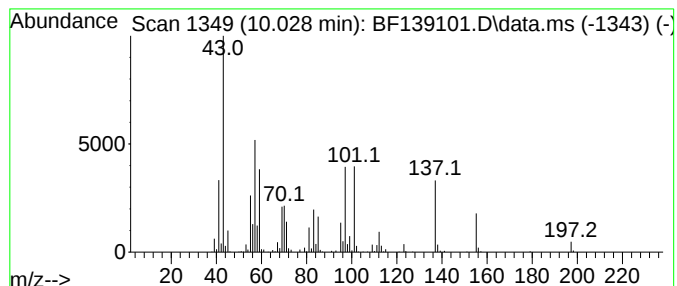
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown10.028 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.028	21.45 ng	902606	Acenaphthene-d10	9.933

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Tetradecanol acetate	256	C16H32O2	051354-23-5	32
2		3-OXO-4-METHYLPENTANOIC ACID, ME...	144	C7H12O3	042558-54-3	16
3		1-Hexadecanol	242	C16H34O	036653-82-4	14
4		Oxirane, [[(2-ethylhexyl)oxy]met...	186	C11H22O2	002461-15-6	10
5		1-Tridecene	182	C13H26	002437-56-1	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139101.D
Acq On : 21 Aug 2024 14:51
Operator : RC/JU
Sample : P3357-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

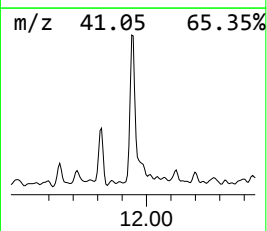
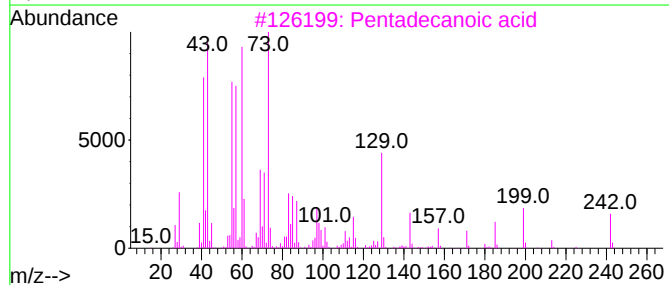
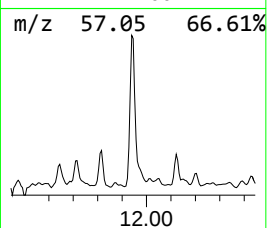
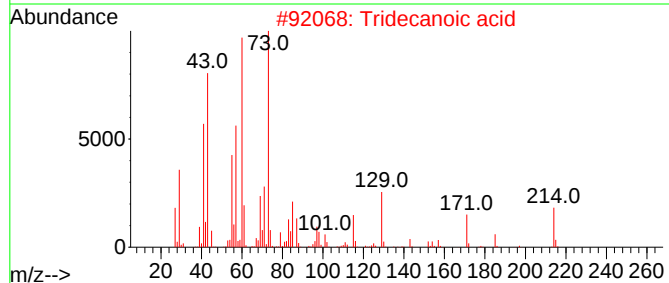
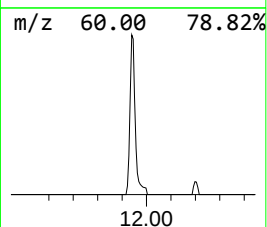
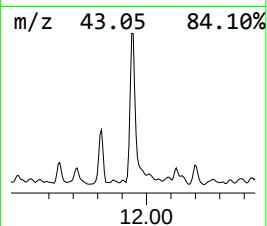
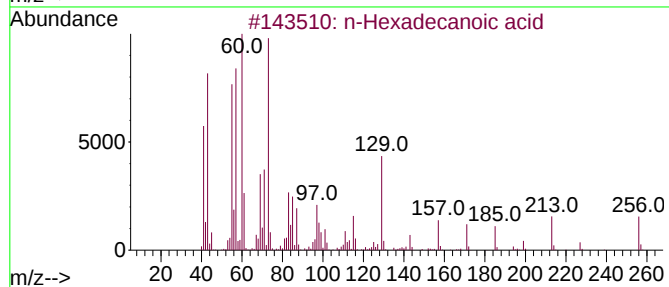
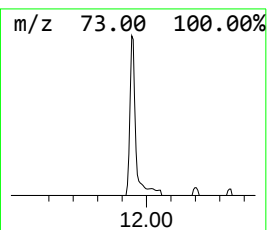
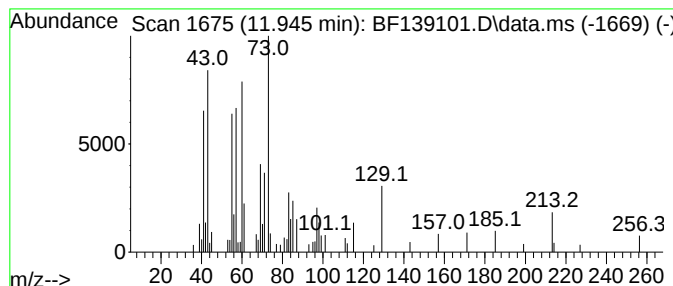
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.945	2.08 ng	75827	Phenanthrene-d10		11.416	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	94
2	Tridecanoic acid		214	C13H26O2	000638-53-9	81
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	74
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	72
5	Lactose		342	C12H22O11	000063-42-3	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139101.D
Acq On : 21 Aug 2024 14:51
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Sample : P3357-05
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ClientSampleId :
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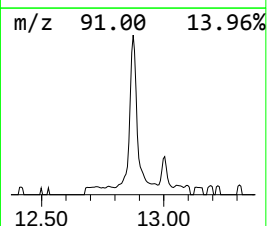
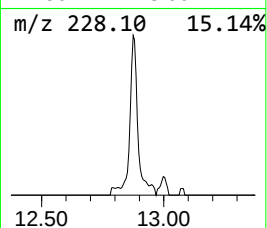
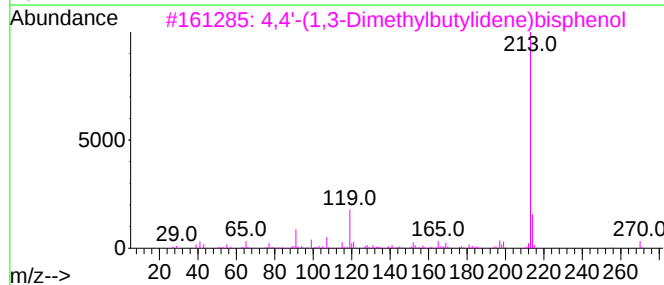
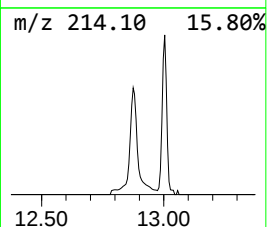
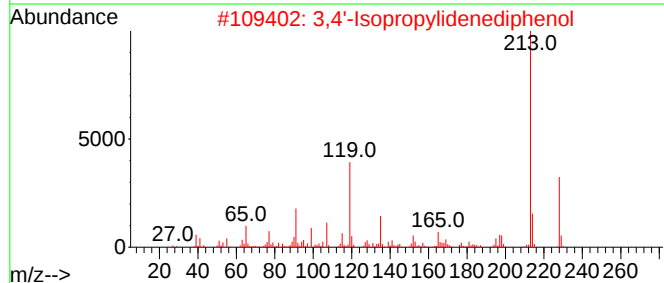
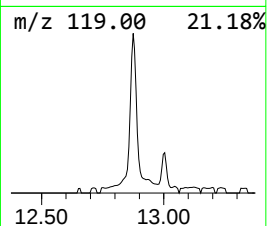
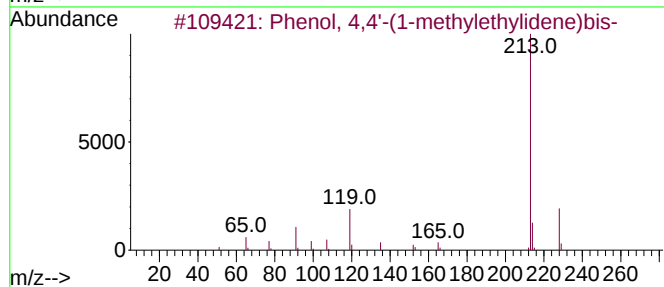
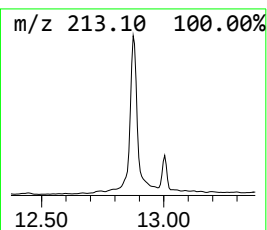
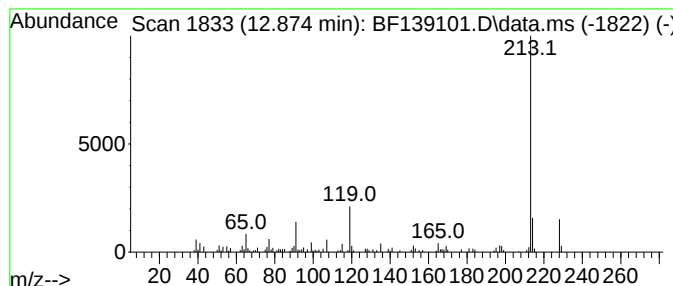
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Phenol, 4,4'-(1-methylethyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.874	6.96 ng	156909	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	96
2			3,4'-Isopropylidenediphenol	228	C15H16O2	046765-25-7	78
3			4,4'-(1,3-Dimethylbutylidene)bis...	270	C18H22O2	006807-17-6	68
4			2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	58
5			6-Bromo-2-(methylamino)troponone	213	C8H8BrNO	1000241-43-1	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139101.D
Acq On : 21 Aug 2024 14:51
Operator : RC/JU
Sample : P3357-05
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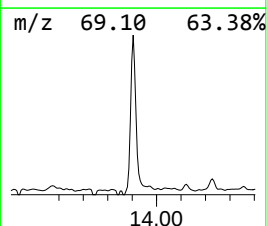
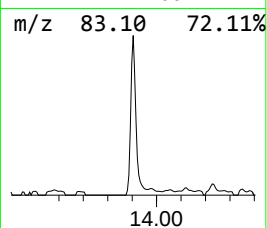
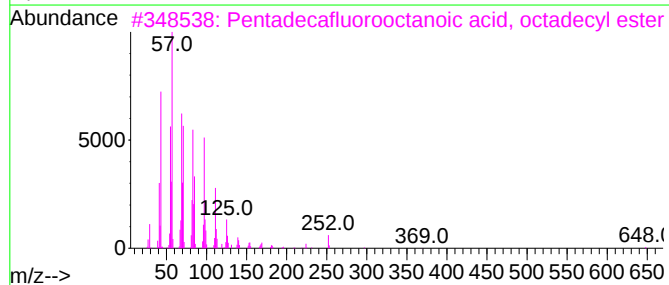
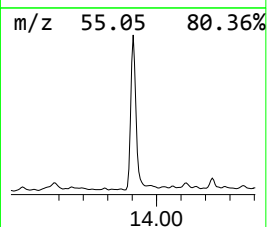
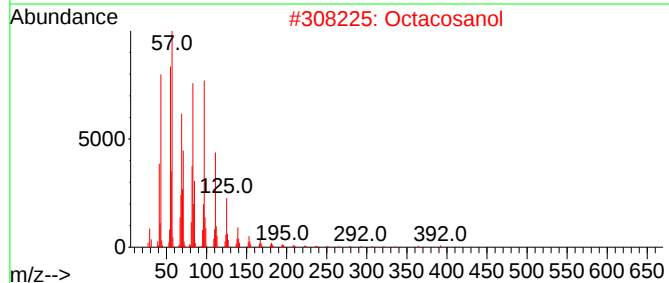
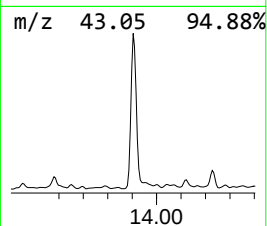
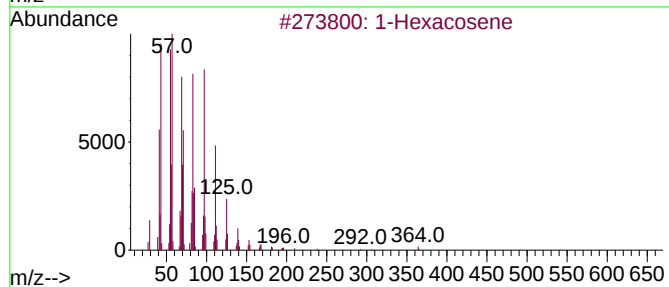
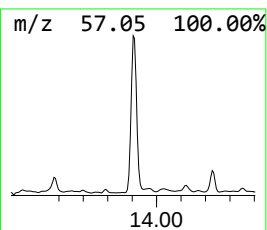
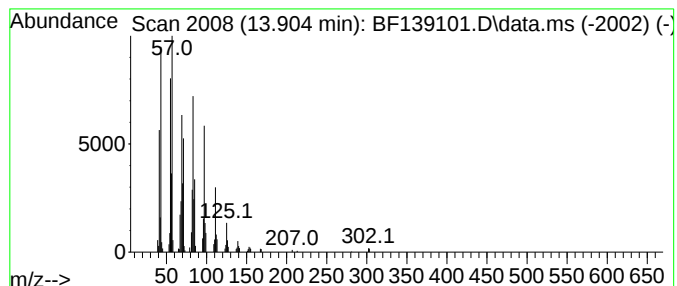
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Hexacosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	7.60 ng	171178	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexacosene	364	C26H52	018835-33-1	94
2			Octacosanol	410	C28H58O	000557-61-9	94
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
4			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
5			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139101.D
Acq On : 21 Aug 2024 14:51
Operator : RC/JU
Sample : P3357-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

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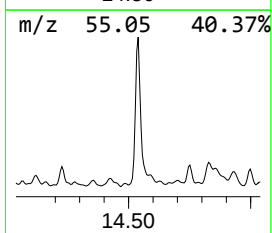
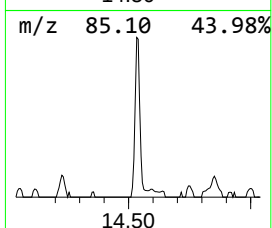
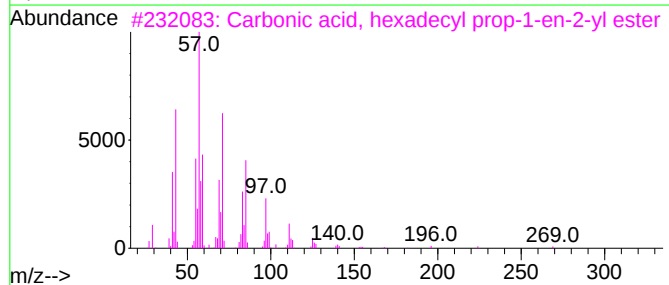
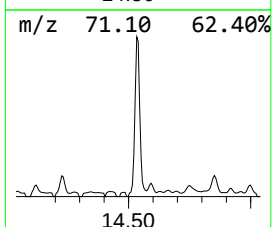
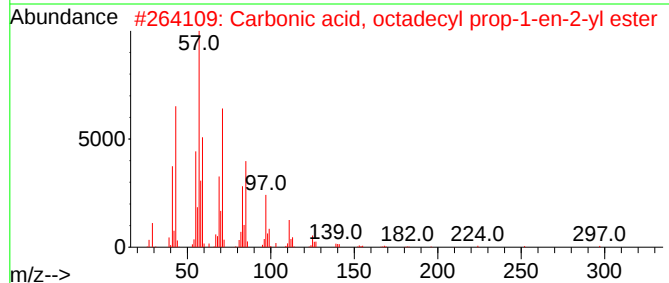
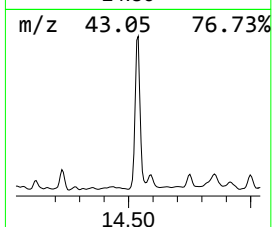
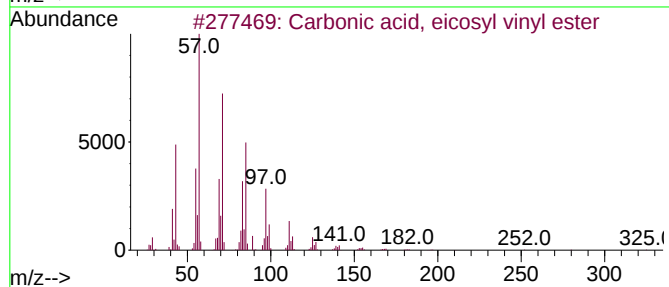
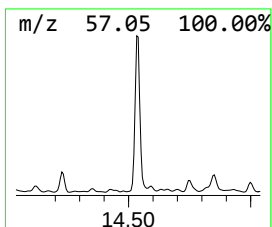
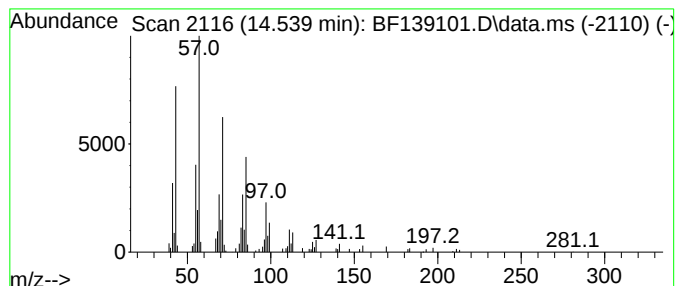
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Carbonic acid, eicosyl vinyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.539	4.91 ng	110582	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	91
2			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	91
3			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	91
4			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	91
5			Tritetracontane	605	C43H88	007098-21-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139101.D
Acq On : 21 Aug 2024 14:51
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Sample : P3357-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

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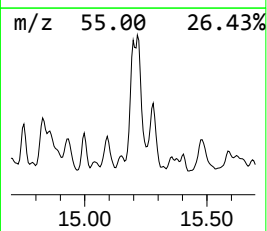
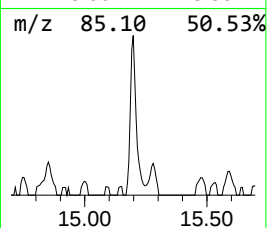
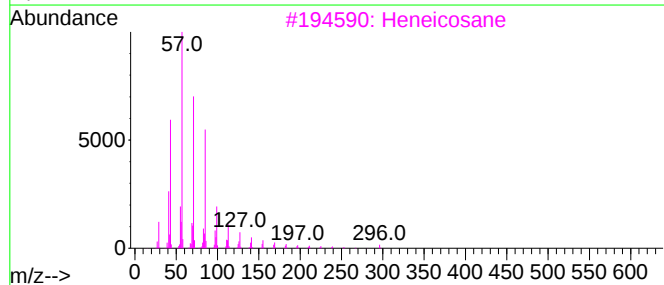
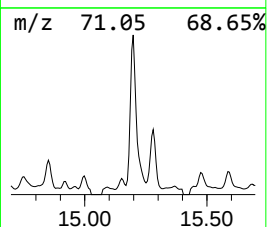
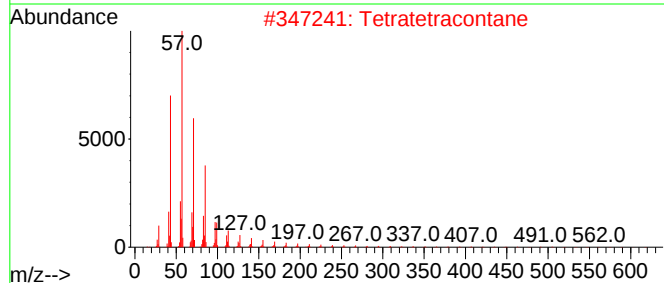
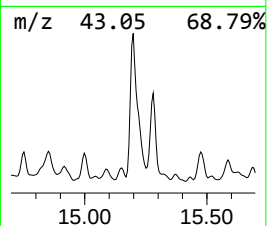
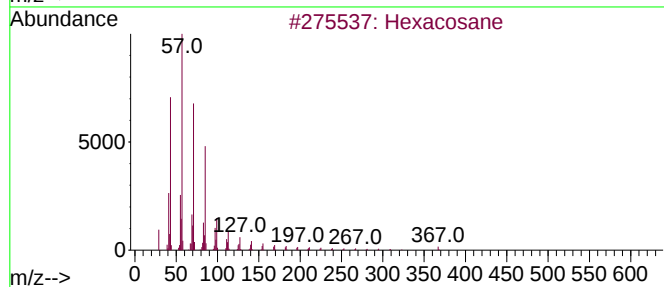
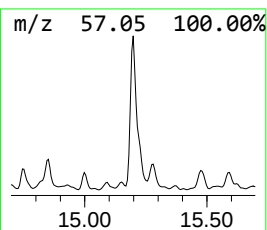
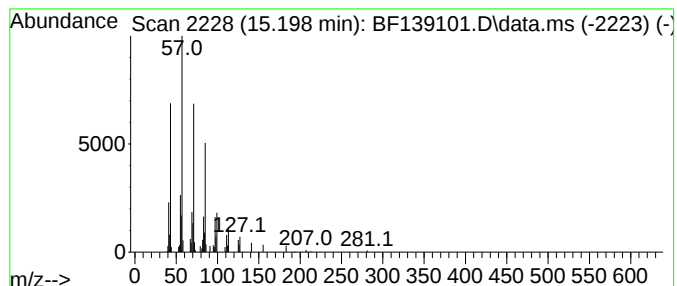
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.198	3.33 ng	87538	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Tetratetracontane	619	C44H90	007098-22-8	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5			Heptadecane	240	C17H36	000629-78-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
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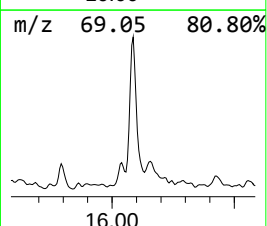
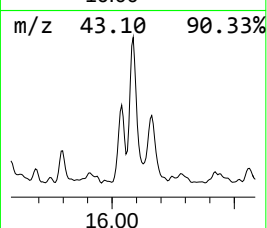
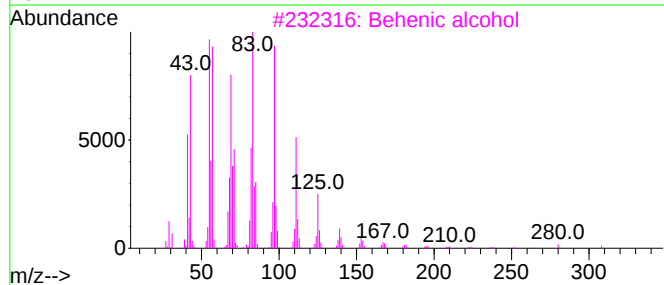
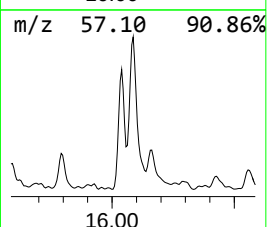
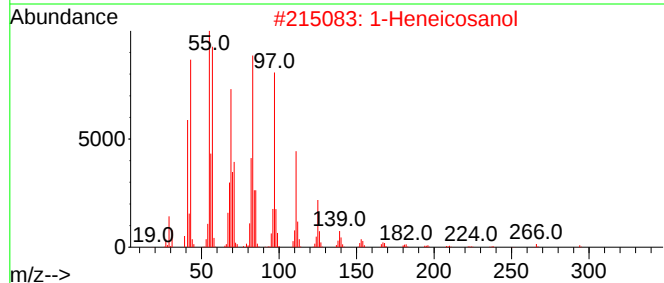
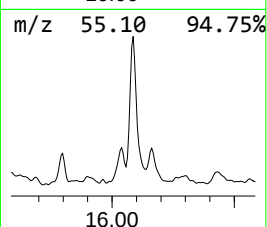
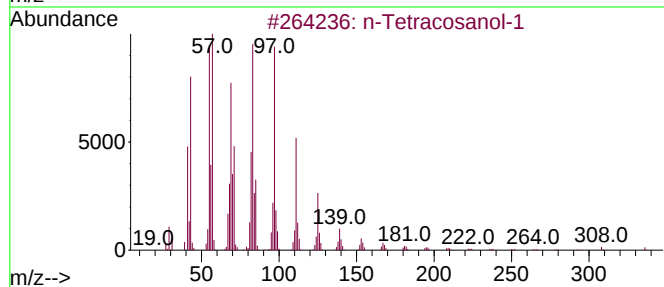
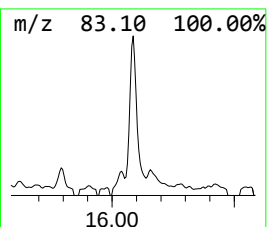
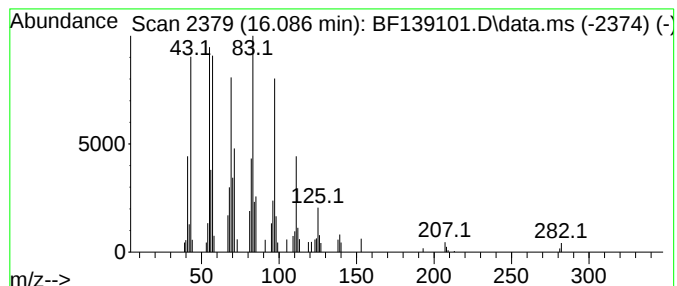
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 n-Tetracosanol-1 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.086	3.75 ng	98625	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2			1-Heneicosanol	312	C21H44O	015594-90-8	95
3			Behenic alcohol	326	C22H46O	000661-19-8	95
4			1-Hexacosene	364	C26H52	018835-33-1	93
5			Octacosanol	410	C28H58O	000557-61-9	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139101.D
Acq On : 21 Aug 2024 14:51
Operator : RC/JU
Sample : P3357-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-857-J-SO-4-4.5-072024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.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	52.9	ng	1552480	1	6.898	586502	20.0
Isopropyl Alcohol	3.404	5.4	ng	157623	1	6.898	586502	20.0
2-Pentanone, 4-...	5.110	4.1	ng	120001	1	6.898	586502	20.0
Ethanol, 2-(2-e...	6.716	2.6	ng	74928	1	6.898	586502	20.0
1-Phenoxypropan...	8.486	4.6	ng	174823	2	8.175	755185	20.0
unknown10.028	10.028	21.4	ng	902606	3	9.933	841438	20.0
n-Hexadecanoic ...	11.945	2.1	ng	75827	4	11.416	729162	20.0
Phenol, 4,4'-(1...	12.874	7.0	ng	156909	5	14.051	450597	20.0
1-Hexacosene	13.904	7.6	ng	171178	5	14.051	450597	20.0
Carbonic acid, ...	14.539	4.9	ng	110582	5	14.051	450597	20.0
Hexacosane	15.198	3.3	ng	87538	6	15.533	525815	20.0
n-Tetracosanol-1	16.086	3.8	ng	98625	6	15.533	525815	20.0