

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082324\
 Data File : BF139150.D
 Acq On : 23 Aug 2024 16:43
 Operator : RC/JU
 Sample : P3707-06
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-913-K1-SO-0.5-1-082024

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: BF139150.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	8	17	24	rVB	910020	1379102	87.86%	10.581%
2	3.399	216	222	249	rBV	41464	103117	6.57%	0.791%
3	5.110	504	513	519	rVB	68034	101956	6.50%	0.782%
4	5.510	575	581	586	rBV	1086591	1391453	88.64%	10.675%
5	6.516	746	752	757	rBV	1097482	1428027	90.97%	10.956%
6	6.716	782	786	792	rBV	31985	39546	2.52%	0.303%
7	6.898	812	817	822	rBV	425231	535769	34.13%	4.111%
8	7.451	906	911	916	rBV	700336	906385	57.74%	6.954%
9	7.710	950	955	960	rVB	31663	37336	2.38%	0.286%
10	8.175	1029	1034	1039	rBV	537698	676541	43.10%	5.191%
11	8.486	1082	1087	1098	rBV	69414	89481	5.70%	0.687%
12	9.251	1212	1217	1222	rBV	1300588	1569713	100.00%	12.043%
13	9.933	1327	1333	1338	rBV	621360	778523	49.60%	5.973%
14	10.028	1343	1349	1357	rVB	31531	46919	2.99%	0.360%
15	10.716	1461	1466	1479	rBV	730322	909687	57.95%	6.979%
16	11.416	1580	1585	1590	rBV	582552	715727	45.60%	5.491%
17	11.939	1670	1674	1689	rBV2	38344	58142	3.70%	0.446%
18	13.004	1849	1855	1860	rVB	1009086	1248213	79.52%	9.577%
19	13.904	2002	2008	2019	rBV2	29209	59798	3.81%	0.459%
20	14.057	2028	2034	2041	rBV	350012	462435	29.46%	3.548%
21	14.921	2177	2181	2188	rVB	12471	17611	1.12%	0.135%
22	15.533	2279	2285	2291	rBV	320481	478626	30.49%	3.672%

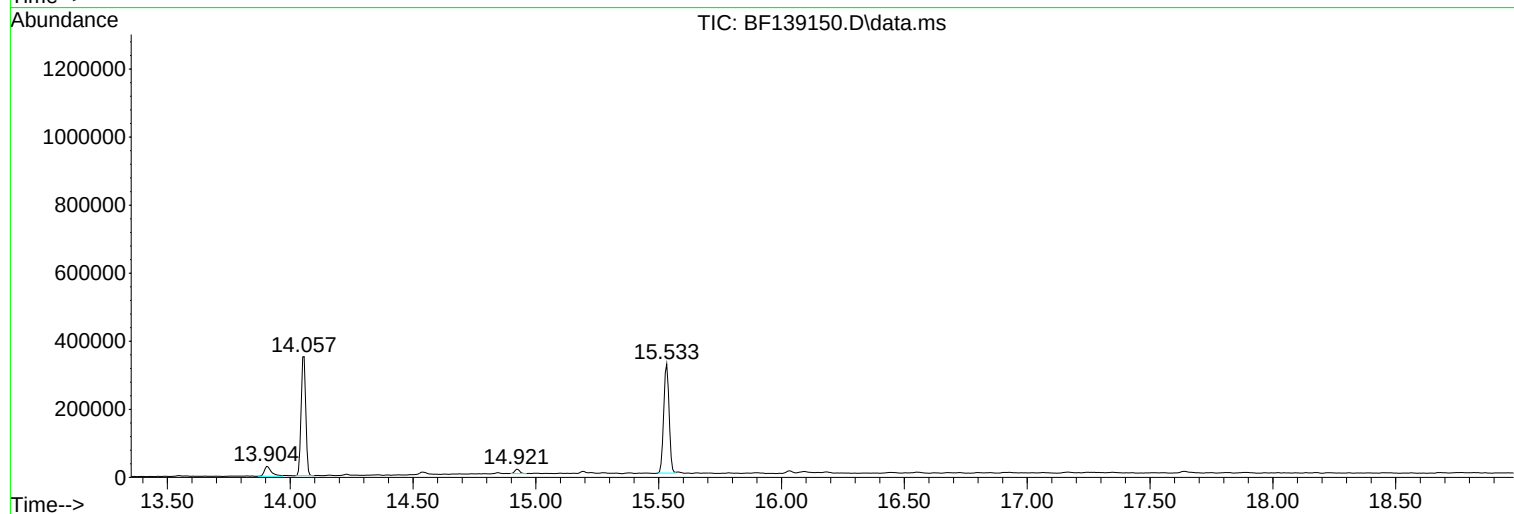
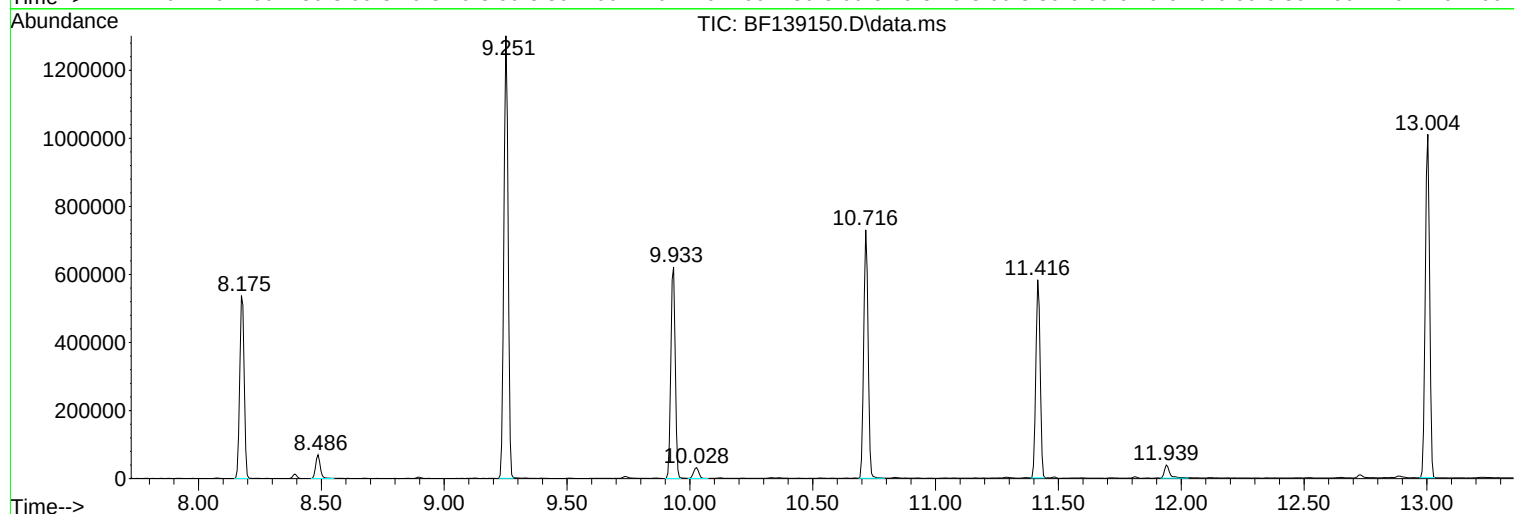
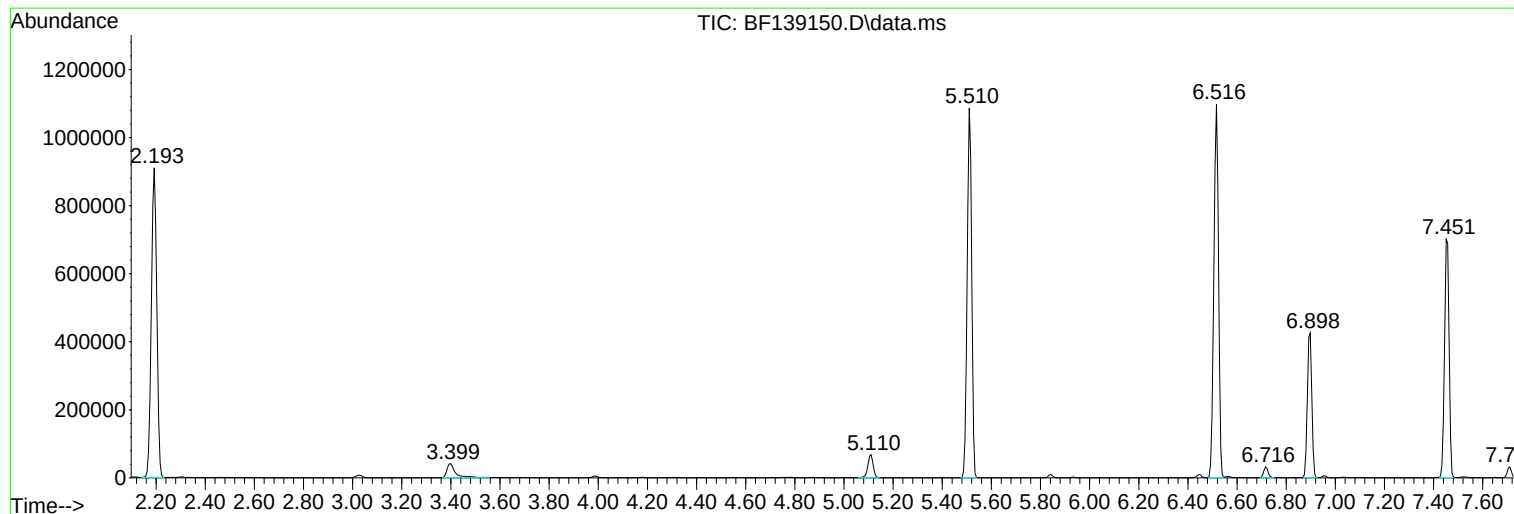
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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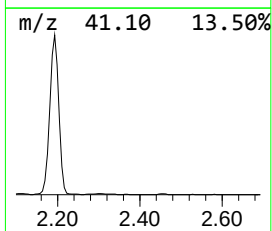
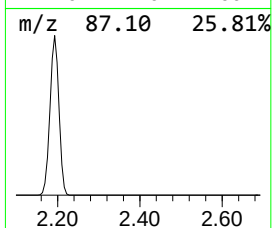
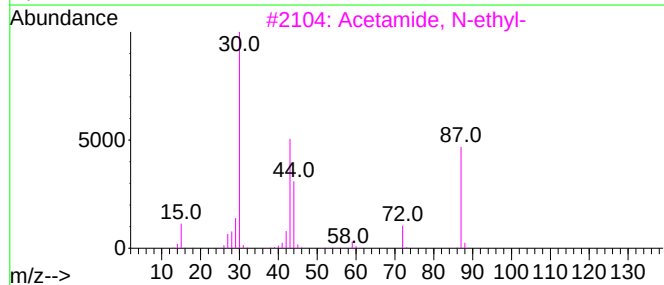
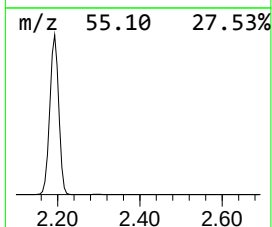
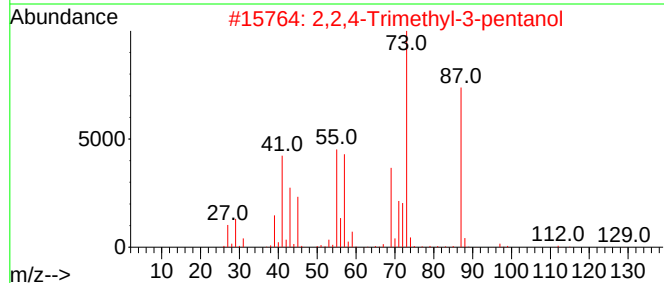
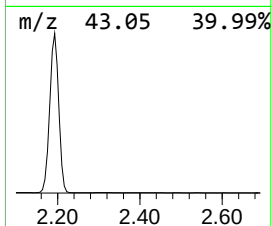
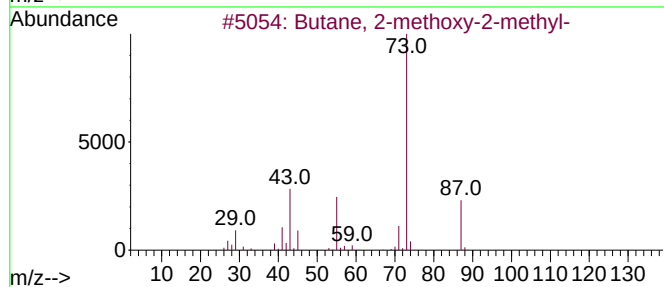
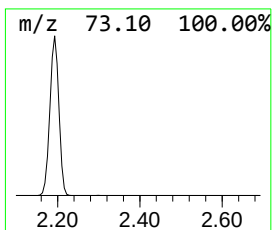
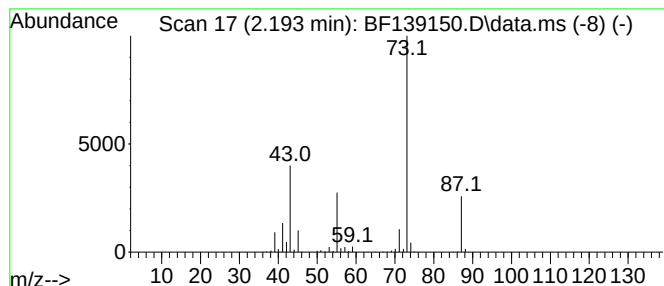
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	51.48 ng	1379100	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			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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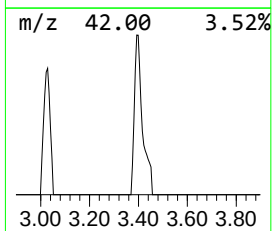
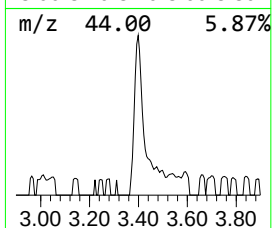
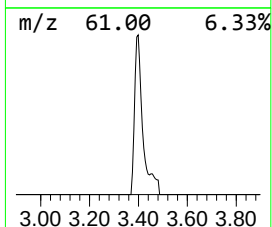
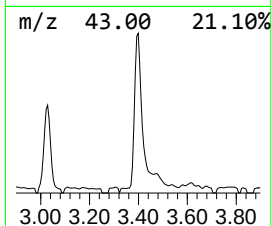
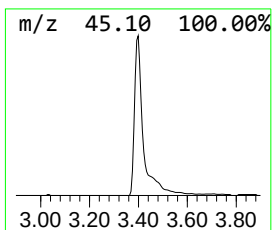
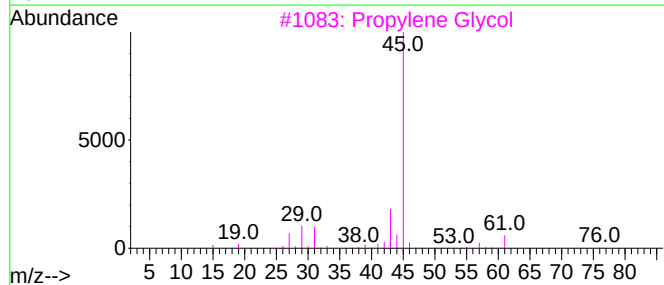
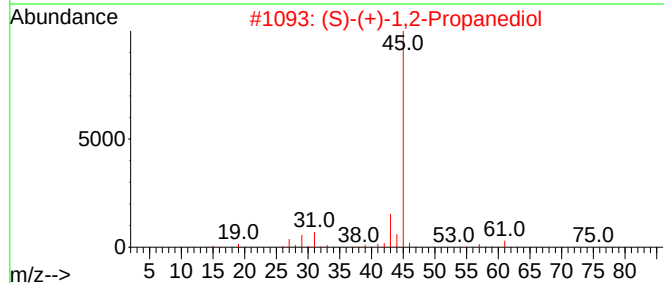
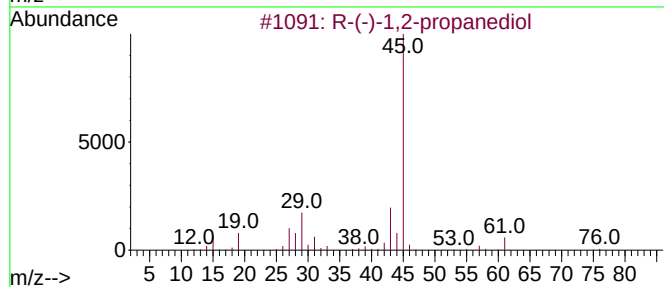
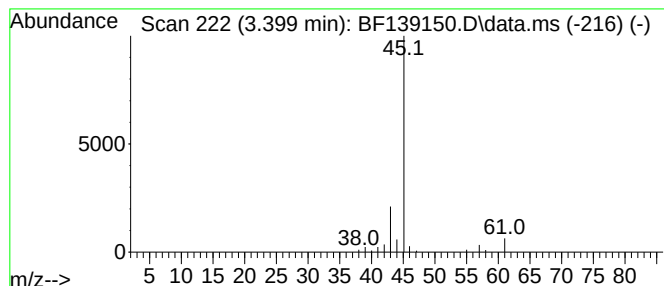
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown3.399 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.399	3.85 ng	103117	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	43
2	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	43
3	Propylene Glycol			76	C3H8O2	000057-55-6	43
4	L-Lactic acid			90	C3H6O3	000079-33-4	9
5	Isopropyl Alcohol			60	C3H8O	000067-63-0	9



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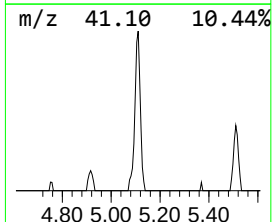
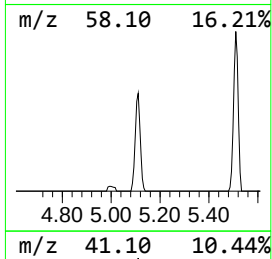
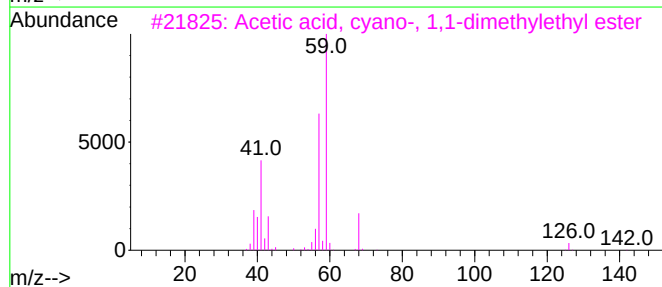
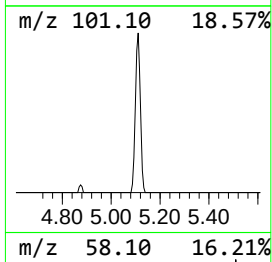
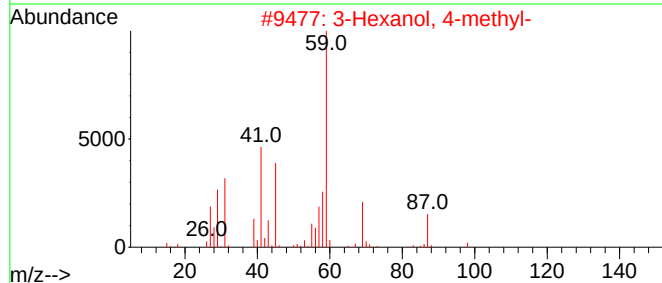
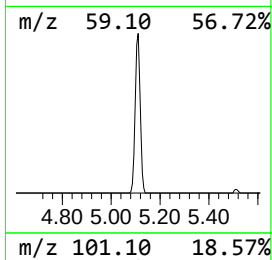
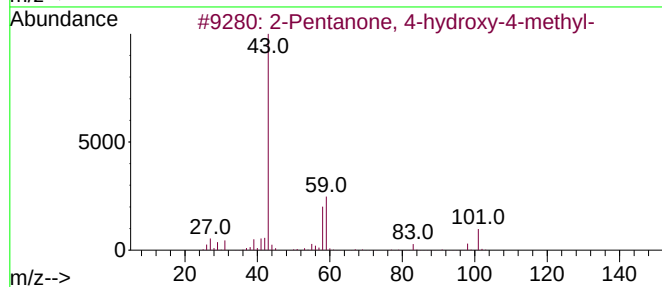
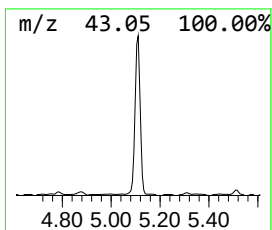
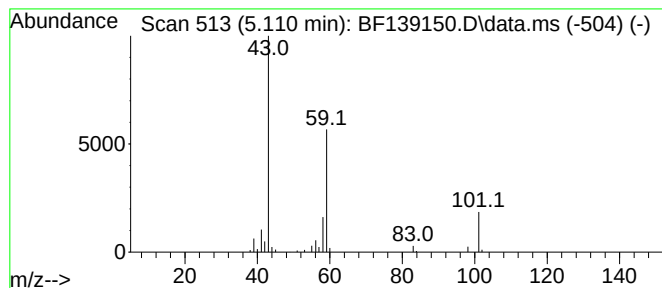
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	3.81 ng	101956	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	50
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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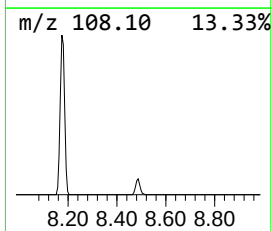
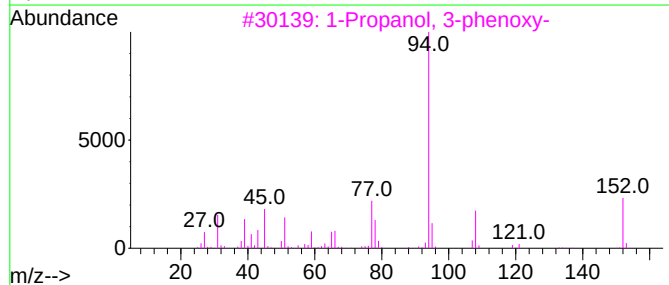
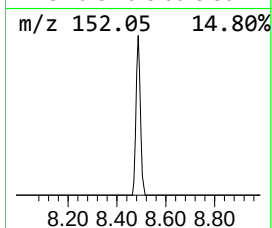
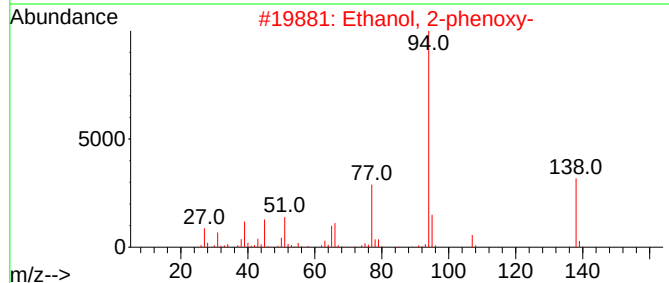
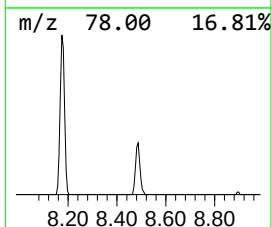
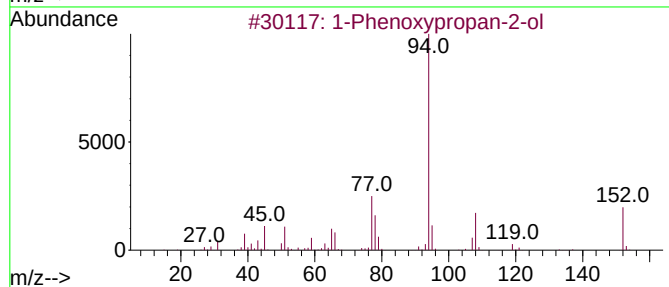
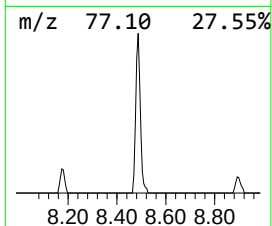
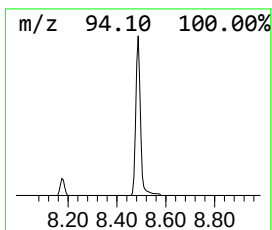
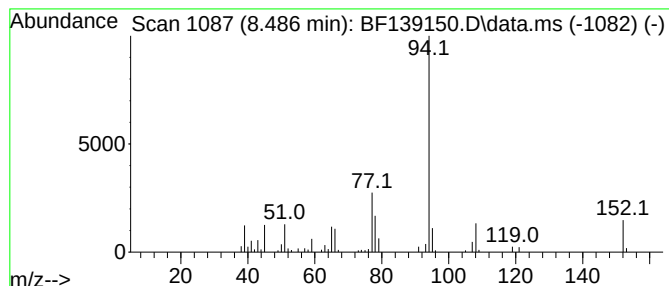
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Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.486	2.65 ng	89481	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			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
3			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	64
4			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
5			Carbonic acid, (3,4,4-trimethyl-...	252	C13H16O5	109123-69-5	59



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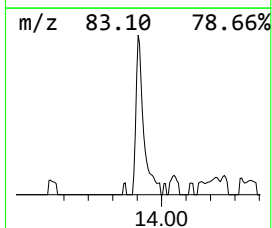
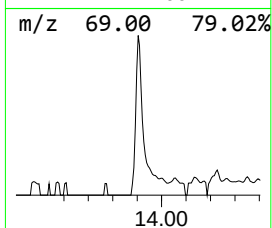
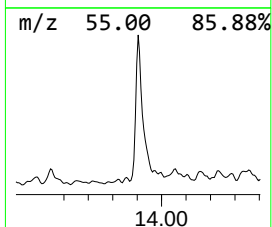
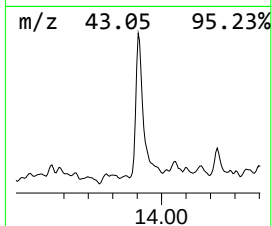
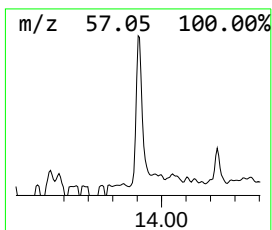
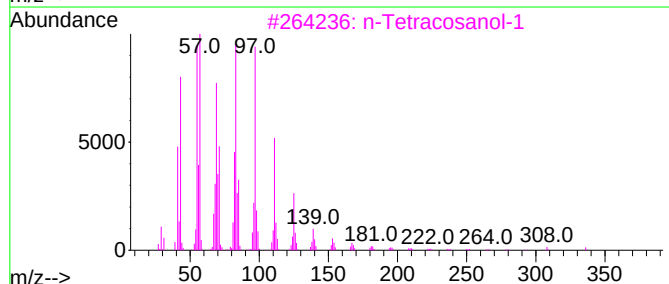
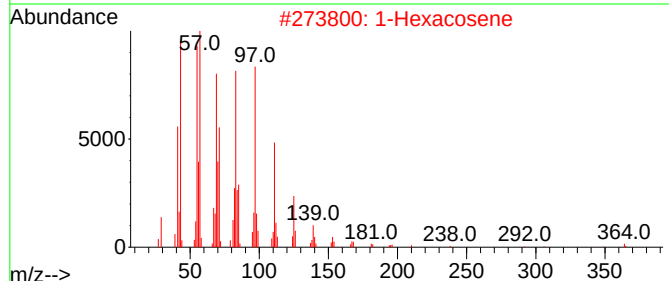
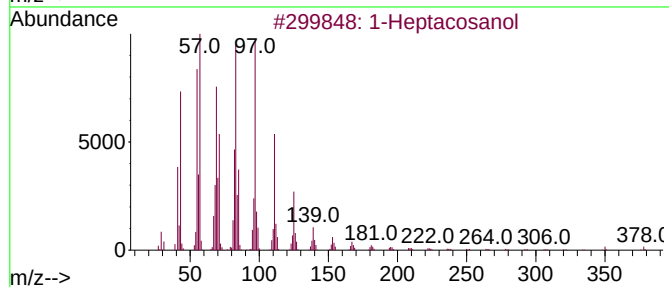
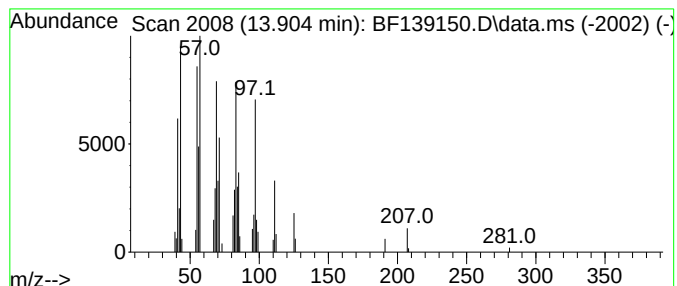
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	2.59 ng	59798	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptacosanol	396	C27H56O	002004-39-9	91
2			1-Hexacosene	364	C26H52	018835-33-1	91
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4			17-Pentatriacontene	491	C35H70	006971-40-0	91
5			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91



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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...	2.193	51.5	ng	1379100	1	6.898	535769	20.0
unknown3.399	3.399	3.9	ng	103117	1	6.898	535769	20.0
2-Pentanone, 4-...	5.110	3.8	ng	101956	1	6.898	535769	20.0
1-Phenoxypropan...	8.486	2.6	ng	89481	2	8.175	676541	20.0
1-Heptacosanol	13.904	2.6	ng	59798	5	14.057	462435	20.0