

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
 Data File : BF138654.D
 Acq On : 25 Jul 2024 15:49
 Operator : RC/JU
 Sample : P3357-03
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-857-J-SO-2-2.5-072024

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-BF070924.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138654.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	3	8	23	rVB	852443	1287360	70.78%	8.092%
2	3.369	213	217	237	rBV	19846	59238	3.26%	0.372%
3	5.075	501	507	520	rVB	87936	129902	7.14%	0.817%
4	5.481	570	576	591	rBV	1320661	1739515	95.63%	10.934%
5	6.487	741	747	766	rBV	1344818	1818911	100.00%	11.433%
6	6.681	773	780	792	rBV	57038	79219	4.36%	0.498%
7	6.851	804	809	814	rBV	393871	483349	26.57%	3.038%
8	7.416	898	905	910	rBV	871202	1150357	63.24%	7.231%
9	7.669	943	948	955	rVB	21004	26684	1.47%	0.168%
10	8.134	1021	1027	1032	rBV	525997	651685	35.83%	4.096%
11	8.445	1075	1080	1094	rBV	129401	183095	10.07%	1.151%
12	9.210	1203	1210	1219	rBV	1375404	1792904	98.57%	11.270%
13	9.886	1320	1325	1330	rBV	593050	725213	39.87%	4.559%
14	9.980	1335	1341	1350	rBV	1049249	1664313	91.50%	10.461%
15	10.675	1454	1459	1475	rBV	864385	1146683	63.04%	7.208%
16	11.374	1572	1578	1587	rBV	542809	710194	39.05%	4.464%
17	11.898	1660	1667	1679	rBV3	26796	54462	2.99%	0.342%
18	12.463	1759	1763	1773	rVB3	19079	30869	1.70%	0.194%
19	12.586	1780	1784	1792	rVB	27595	34903	1.92%	0.219%
20	12.816	1817	1823	1826	rBV	20083	28207	1.55%	0.177%
21	12.957	1841	1847	1852	rBV	928771	1214876	66.79%	7.636%
22	13.851	1993	1999	2015	rBV2	38765	87082	4.79%	0.547%
23	14.010	2021	2026	2035	rVB	284908	375714	20.66%	2.362%
24	14.468	2100	2104	2108	rBV	16284	24527	1.35%	0.154%
25	15.045	2199	2202	2210	rBV	8596	19335	1.06%	0.122%
26	15.474	2269	2275	2287	rVB	253558	390352	21.46%	2.454%

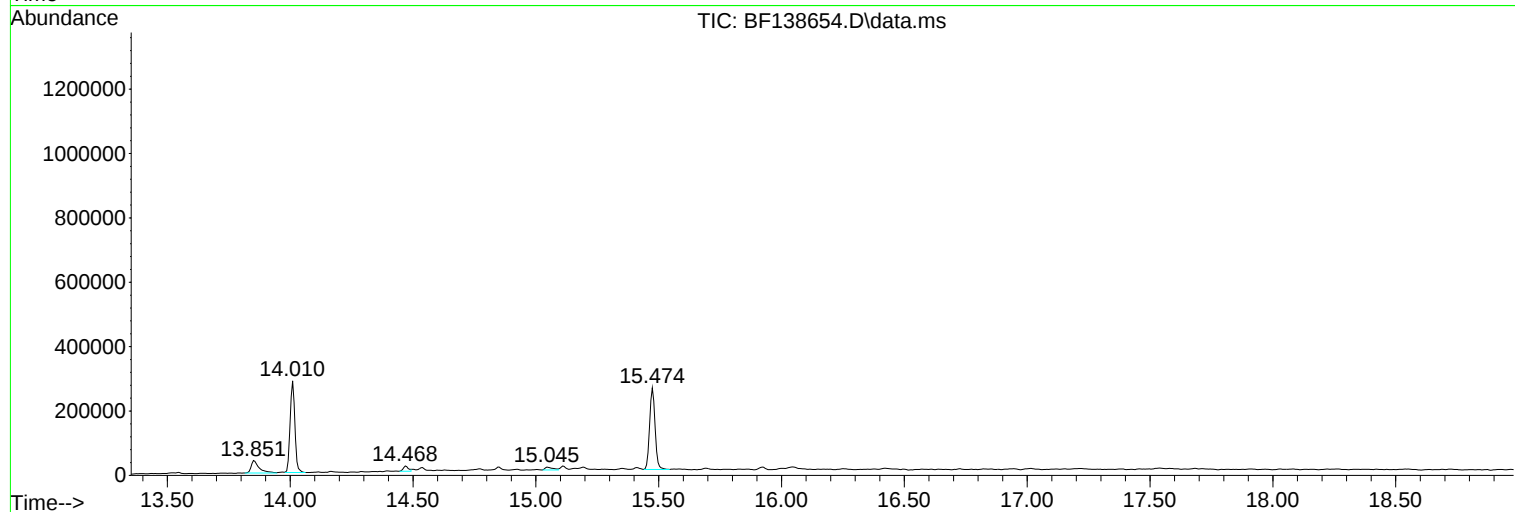
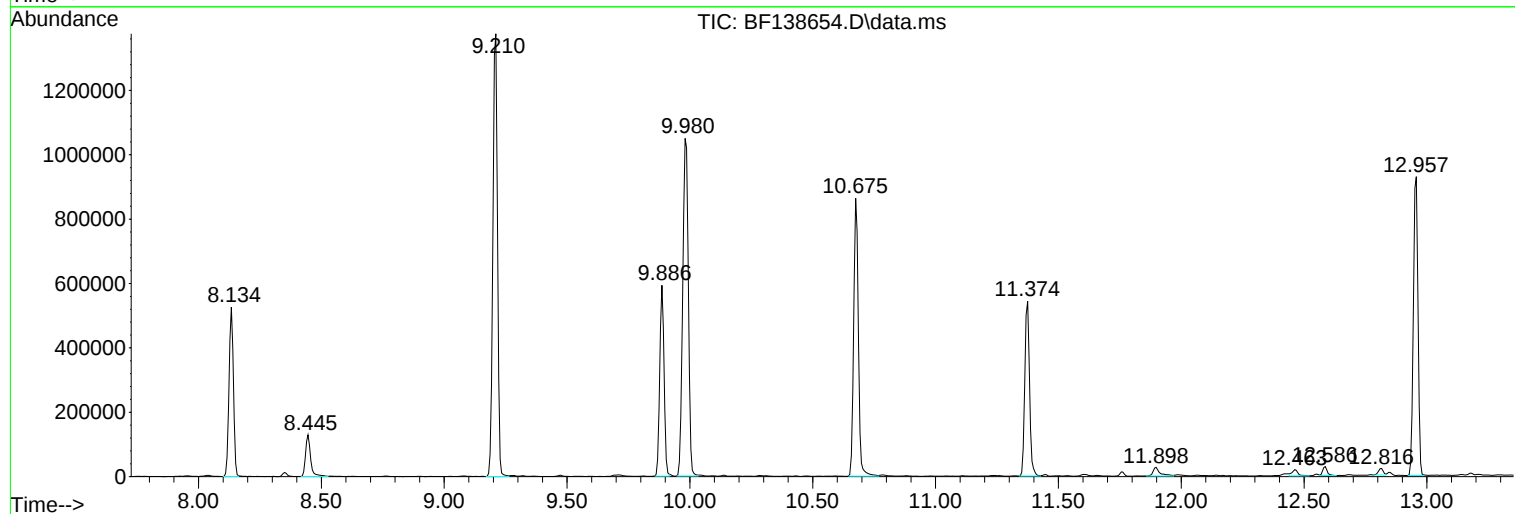
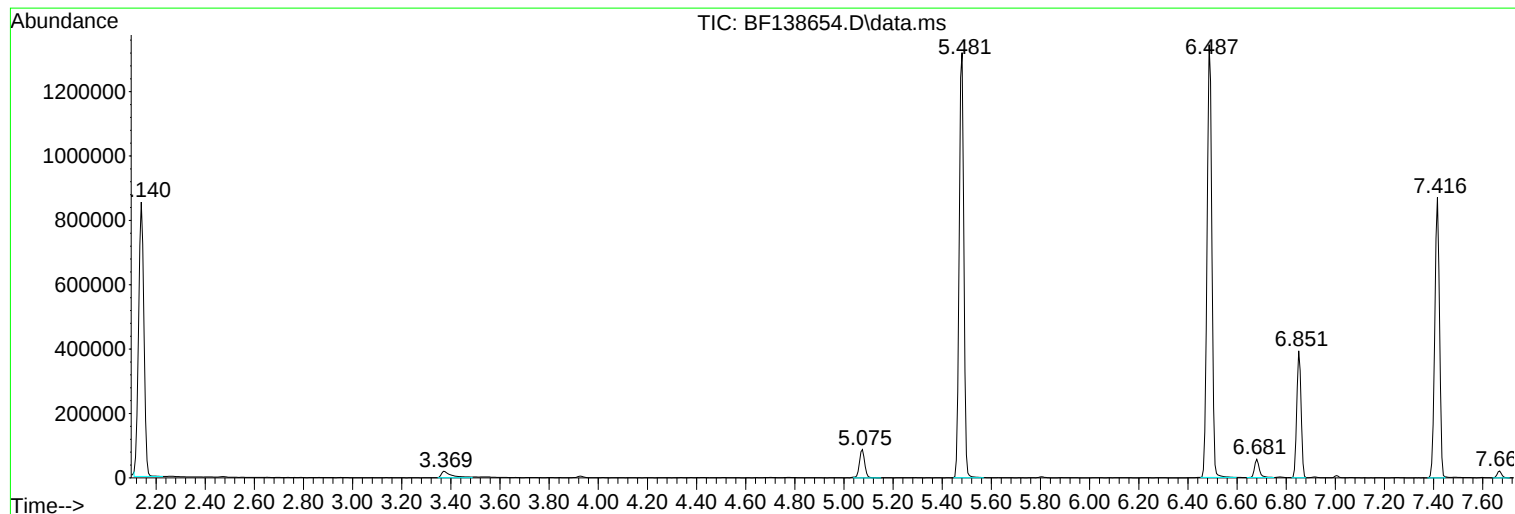
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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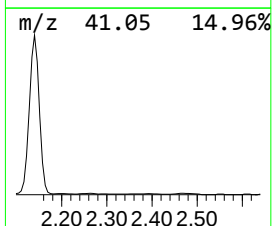
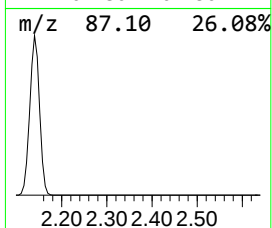
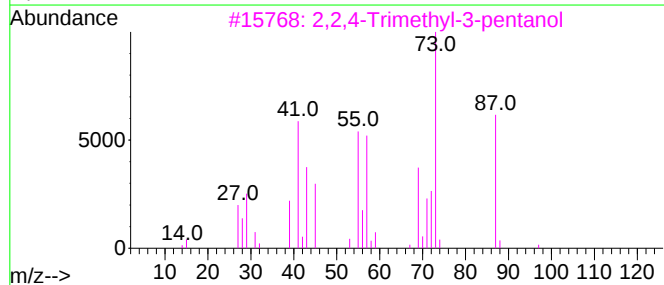
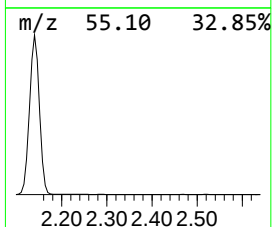
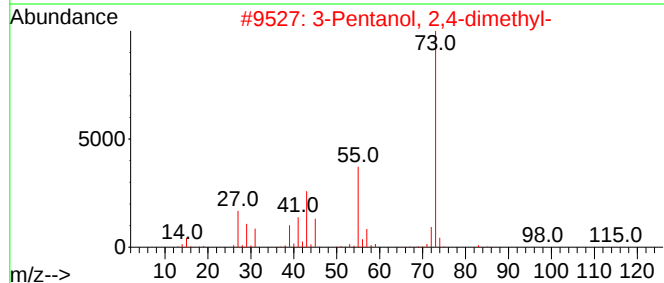
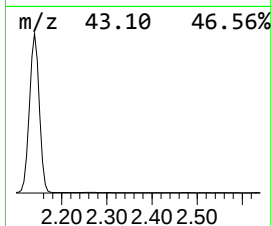
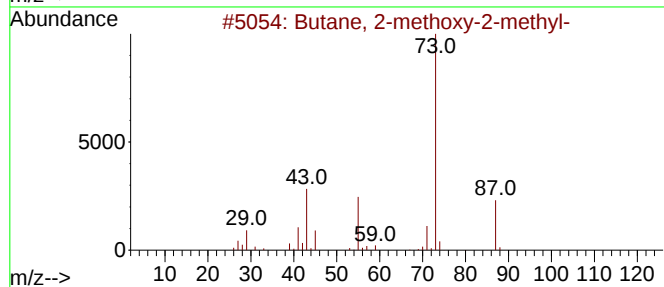
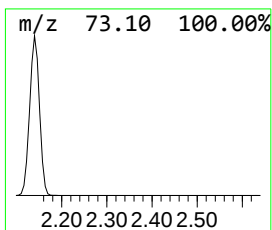
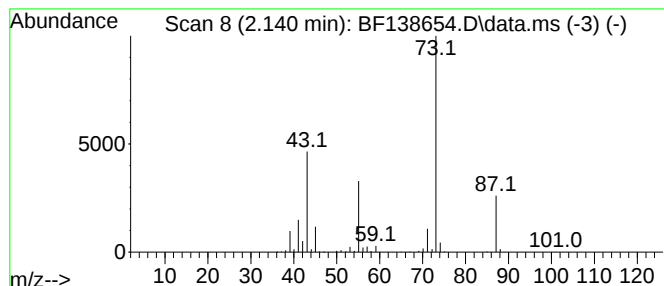
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	53.27 ng	1287360	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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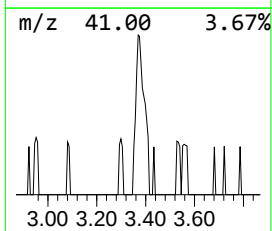
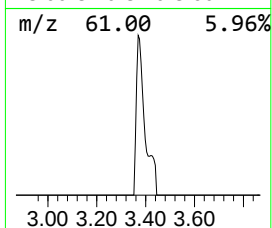
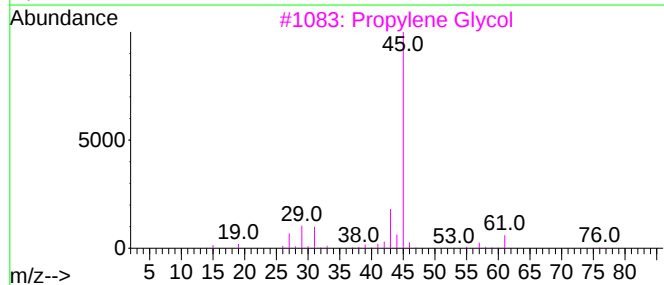
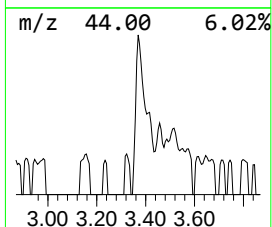
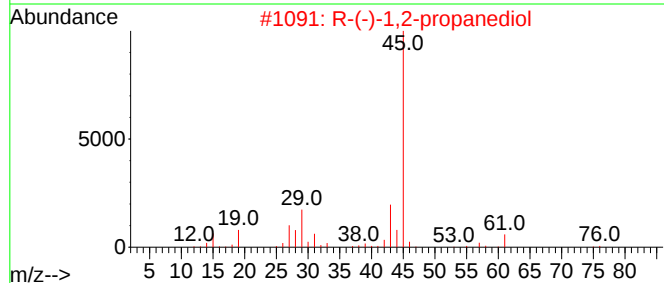
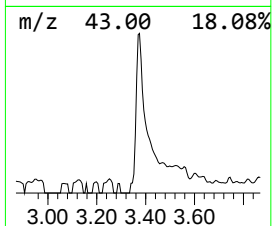
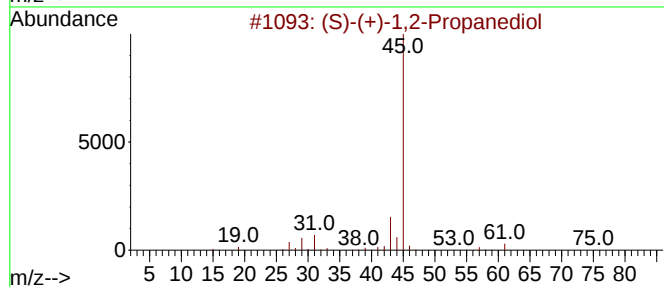
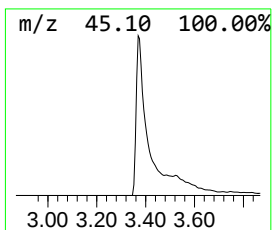
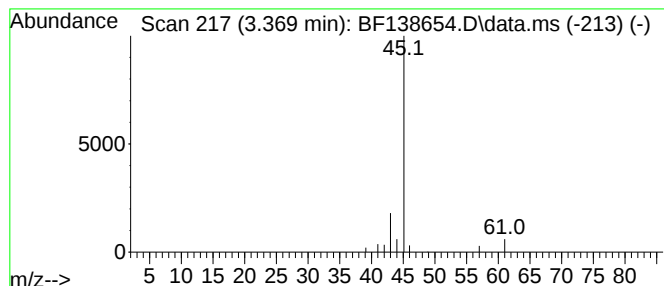
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Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.369	2.45 ng	59238	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	74
2	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	64
3	Propylene Glycol			76	C3H8O2	000057-55-6	9
4	Formamide			45	CH3NO	000075-12-7	7
5	Propanoic acid, 2-hydroxy-, meth...			104	C4H8O3	000547-64-8	4



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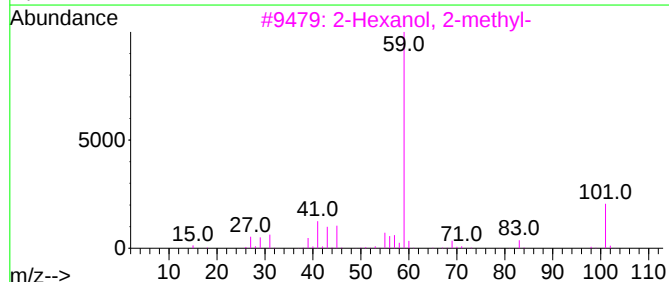
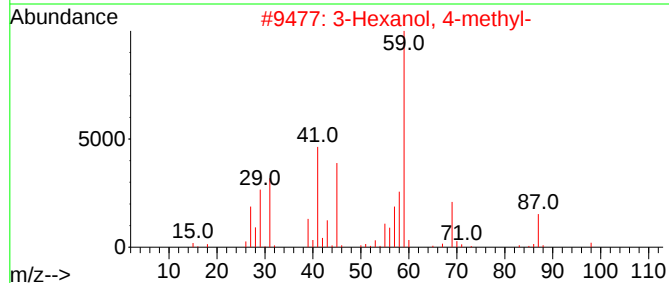
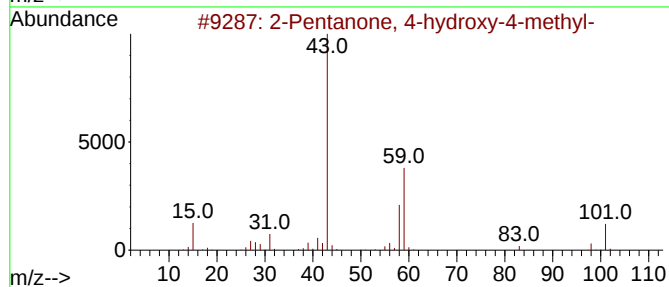
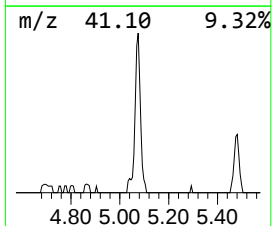
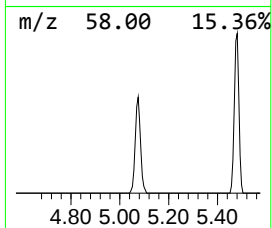
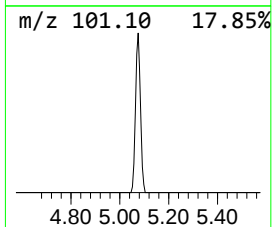
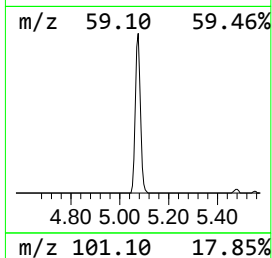
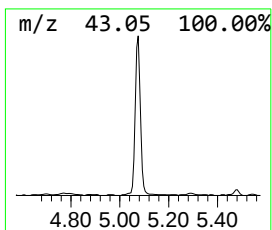
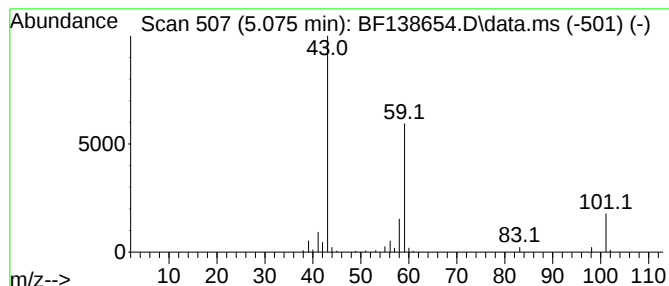
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	5.38 ng	129902	1,4-Dichlorobenzene-d4	6.851

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			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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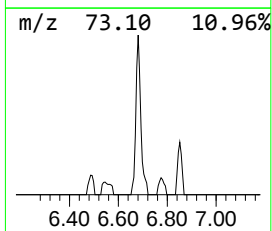
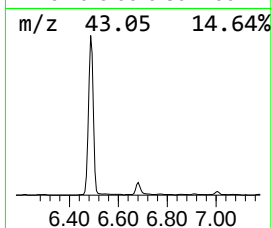
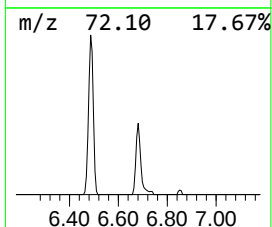
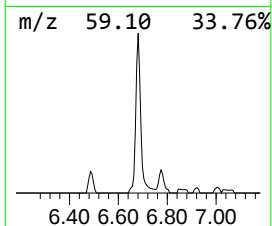
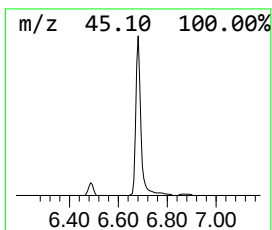
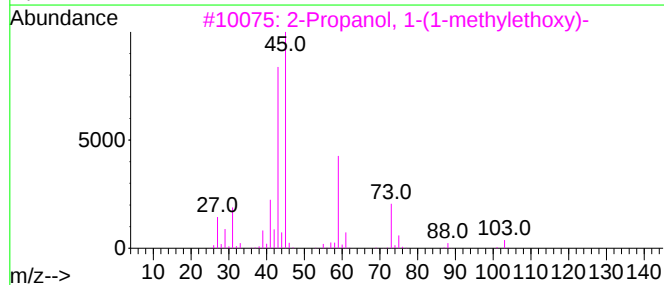
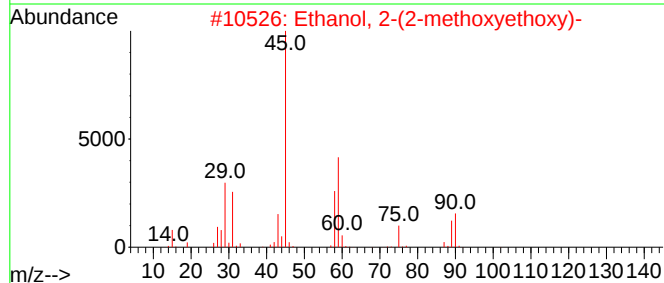
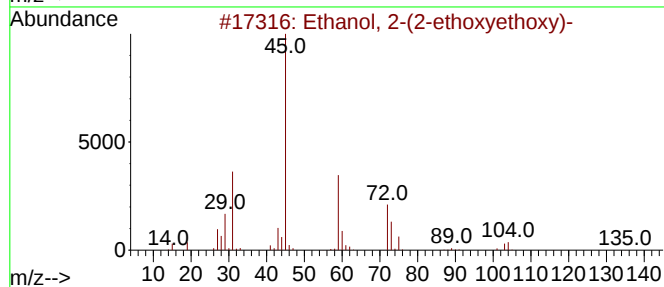
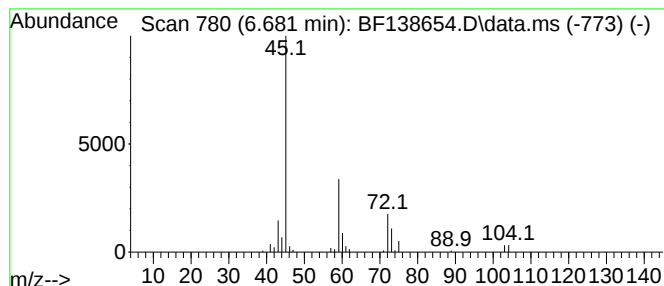
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Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.681	3.28 ng	79219	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	50
3			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	39
4			Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	38
5			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	37



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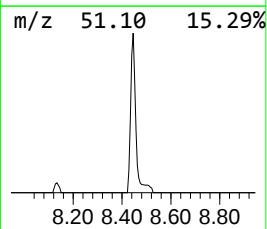
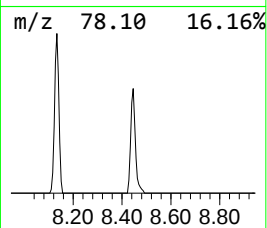
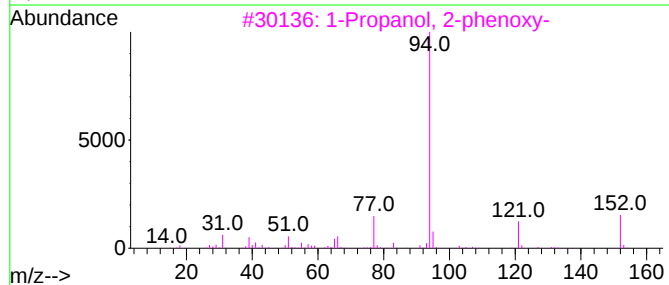
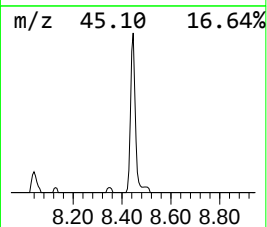
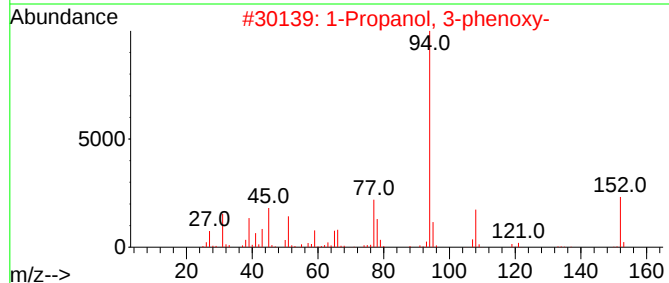
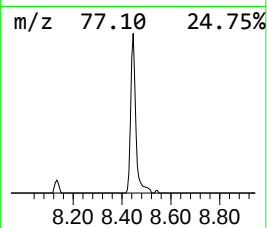
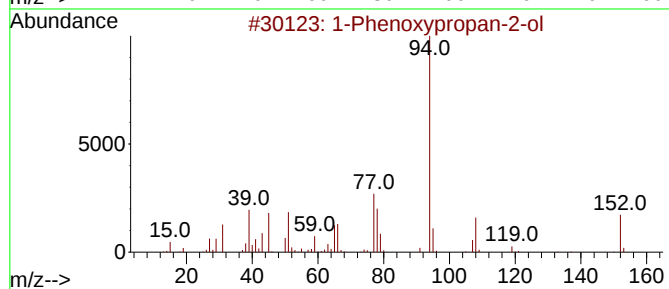
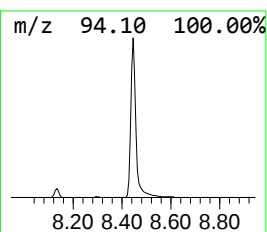
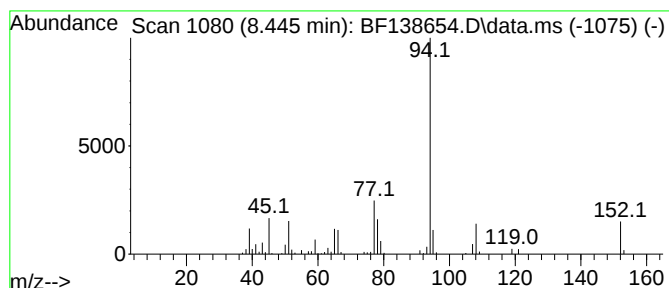
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Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.445	5.62 ng	183095	Naphthalene-d8	8.134

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	74
3			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
5			Benzene, (1-methylpropoxy)-	150	C10H14O	010574-17-1	53



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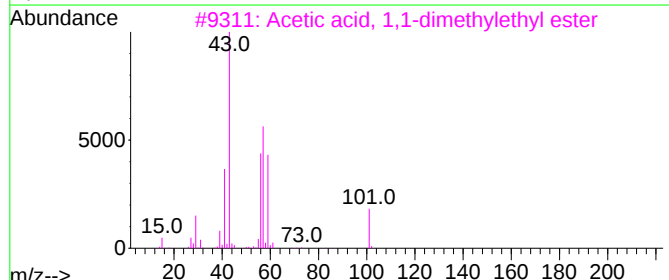
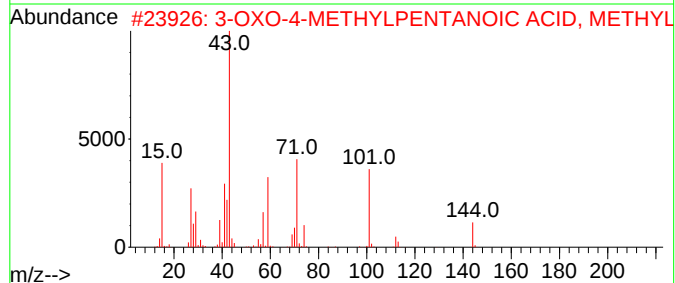
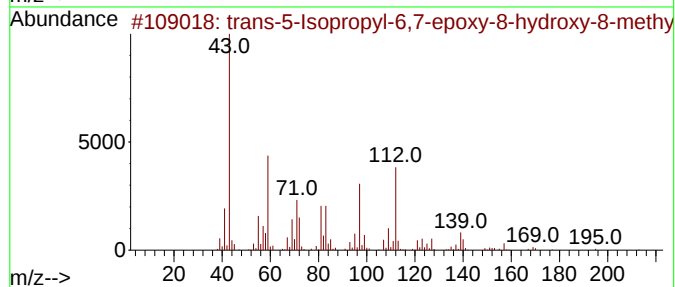
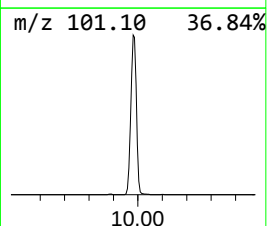
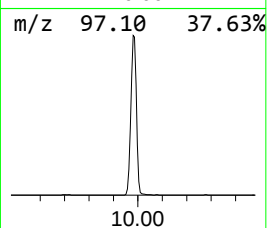
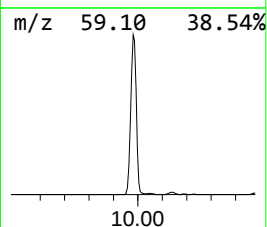
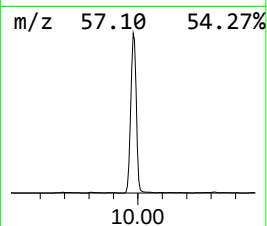
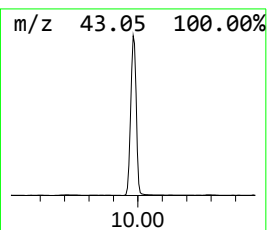
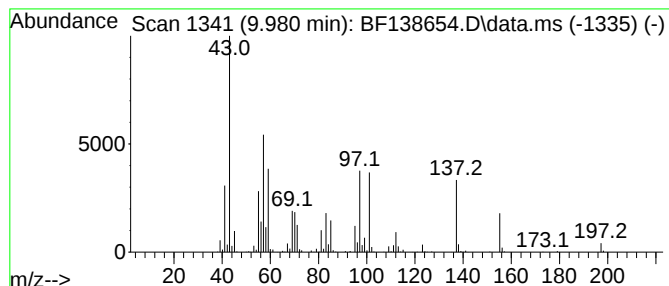
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown9.980 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.980	45.90 ng	1664310	Acenaphthene-d10	9.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	32
2			3-OXO-4-METHYLPENTANOIC ACID, ME...	144	C7H12O3	042558-54-3	25
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	16
4			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	12
5			2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
Data File : BF138654.D
Acq On : 25 Jul 2024 15:49
Operator : RC/JU
Sample : P3357-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-857-J-SO-2-2.5-072024

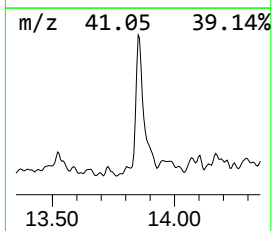
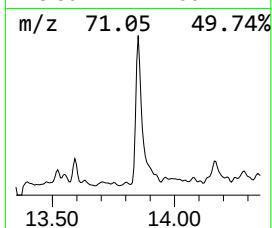
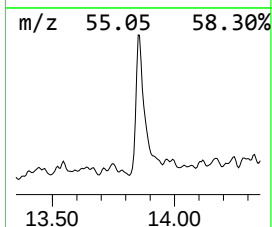
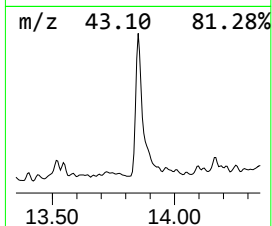
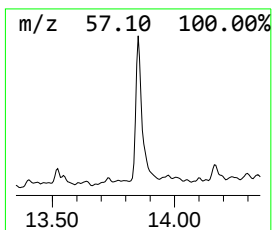
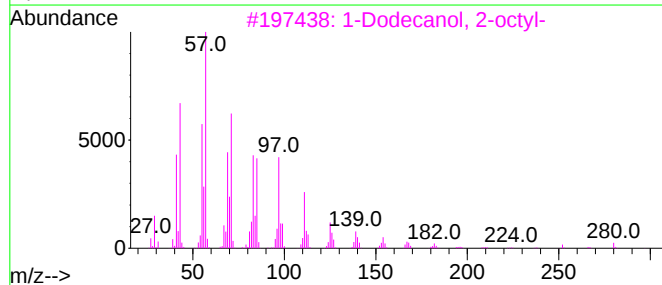
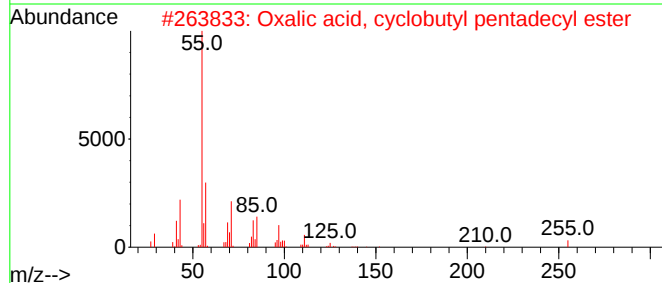
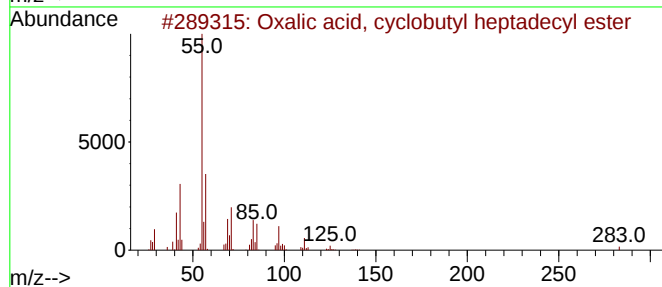
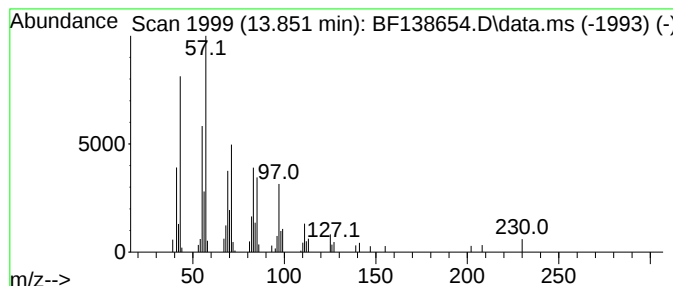
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Oxalic acid, cyclobutyl hep... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	4.64 ng	87082	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	91
2			Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1010309-70-5	91
3			1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
4			Oxalic acid, cyclobutyl hexadecy...	368	C22H40O4	1000309-70-6	90
5			Oxalic acid, cyclobutyl octadecy...	396	C24H44O4	1000309-70-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
Data File : BF138654.D
Acq On : 25 Jul 2024 15:49
Operator : RC/JU
Sample : P3357-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-857-J-SO-2-2.5-072024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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...	2.140	53.3	ng	1287360	1	6.851	483349	20.0
(S)-(+)-1,2-Pro...	3.369	2.5	ng	59238	1	6.851	483349	20.0
2-Pentanone, 4-...	5.075	5.4	ng	129902	1	6.851	483349	20.0
Ethanol, 2-(2-e...	6.681	3.3	ng	79219	1	6.851	483349	20.0
1-Phenoxypropan...	8.445	5.6	ng	183095	2	8.134	651685	20.0
unknown9.980	9.980	45.9	ng	1664310	3	9.886	725213	20.0
Oxalic acid, cy...	13.851	4.6	ng	87082	5	14.010	375714	20.0