

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
 Data File : BF138657.D
 Acq On : 25 Jul 2024 17:20
 Operator : RC/JU
 Sample : P3357-09
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-854-J-SO-3-3.5-072024

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: BF138657.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.157	3	11	23	rVB	979928	1541246	49.11%	8.871%
2	3.381	214	219	237	rBV	29102	77808	2.48%	0.448%
3	5.075	498	507	517	rVB	87478	128075	4.08%	0.737%
4	5.481	570	576	587	rBV	1328276	1702892	54.26%	9.801%
5	6.487	741	747	771	rVB	1332073	1775525	56.57%	10.219%
6	6.681	775	780	792	rVB	47903	65783	2.10%	0.379%
7	6.851	804	809	814	rVB	332566	400628	12.76%	2.306%
8	7.416	898	905	910	rBV	867919	1159009	36.93%	6.671%
9	8.133	1021	1027	1036	rBV	433150	570658	18.18%	3.284%
10	8.445	1075	1080	1095	rBV	86779	126376	4.03%	0.727%
11	9.204	1203	1209	1214	rBV	1503594	1957014	62.35%	11.263%
12	9.886	1319	1325	1329	rBV	481027	601954	19.18%	3.465%
13	9.986	1334	1342	1353	rBV	1938598	3138555	100.00%	18.064%
14	10.674	1454	1459	1474	rBV	886992	1147562	36.56%	6.605%
15	11.369	1572	1577	1586	rBV2	452435	643181	20.49%	3.702%
16	11.898	1659	1667	1678	rBV4	19358	40257	1.28%	0.232%
17	12.416	1744	1755	1759	rBV4	16047	32977	1.05%	0.190%
18	12.463	1759	1763	1772	rVB3	21972	36262	1.16%	0.209%
19	12.580	1780	1783	1786	rBV	33673	39252	1.25%	0.226%
20	12.810	1817	1822	1826	rBV	26973	36757	1.17%	0.212%
21	12.951	1841	1846	1851	rBV	1103611	1399875	44.60%	8.057%
22	13.851	1994	1999	2016	rBV	45630	107430	3.42%	0.618%
23	14.004	2020	2025	2033	rVB	230508	319682	10.19%	1.840%
24	15.468	2268	2274	2284	rVB	204802	326158	10.39%	1.877%

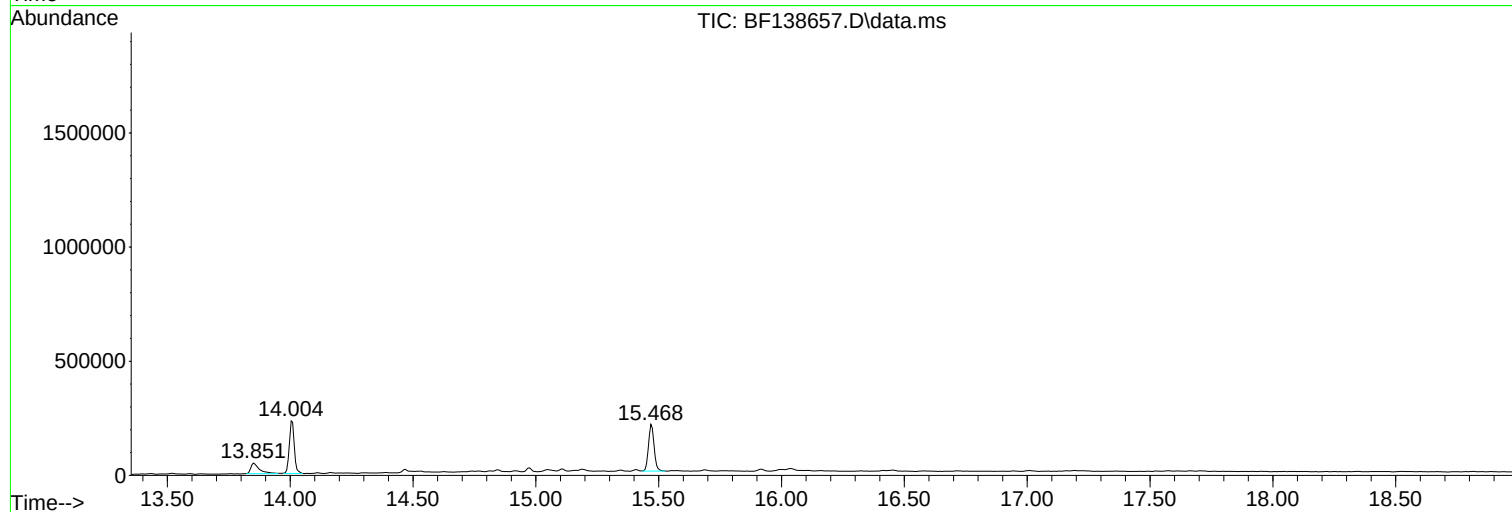
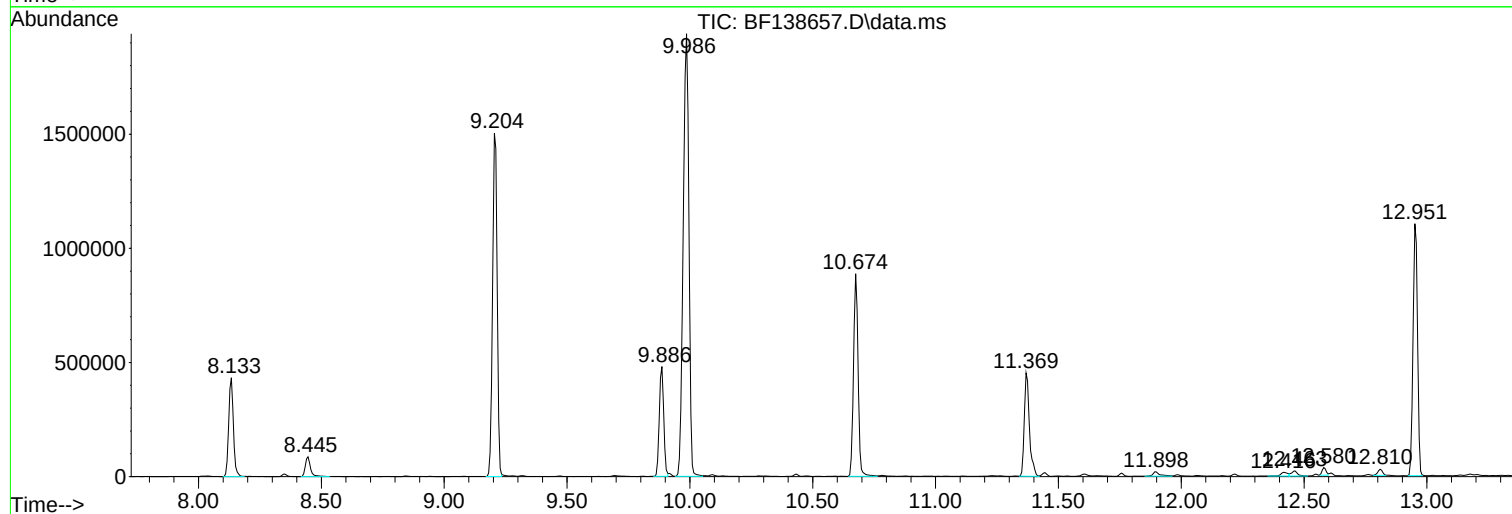
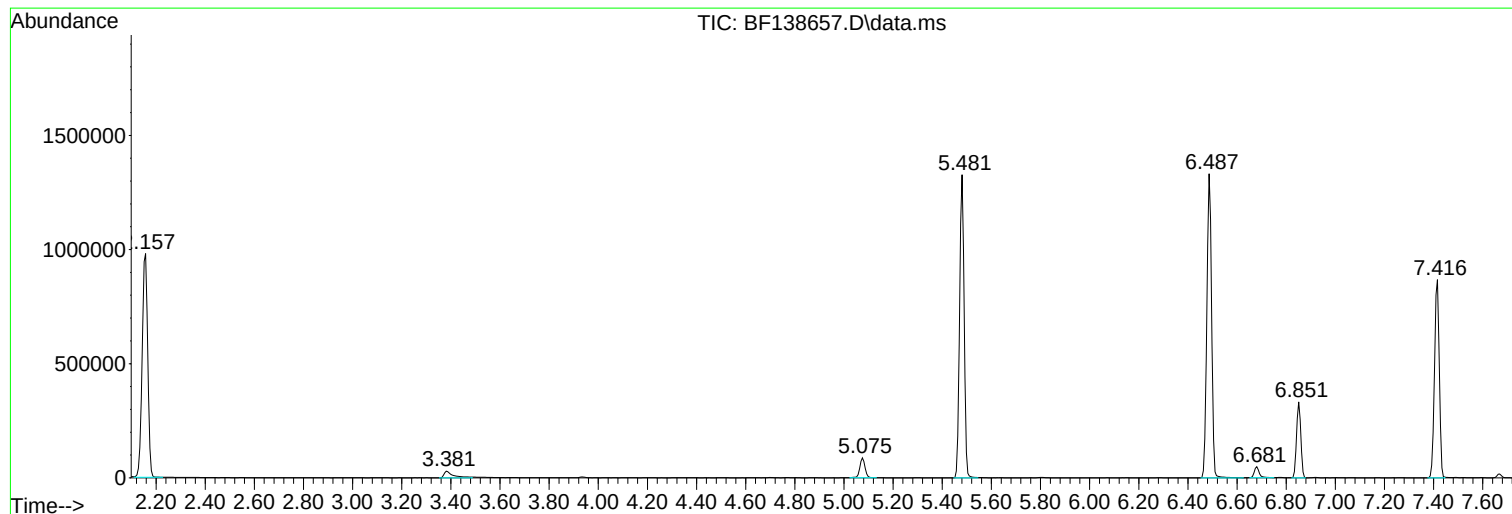
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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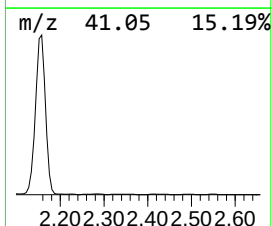
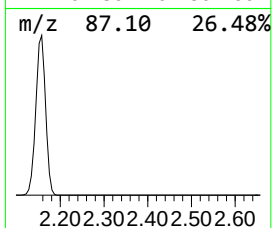
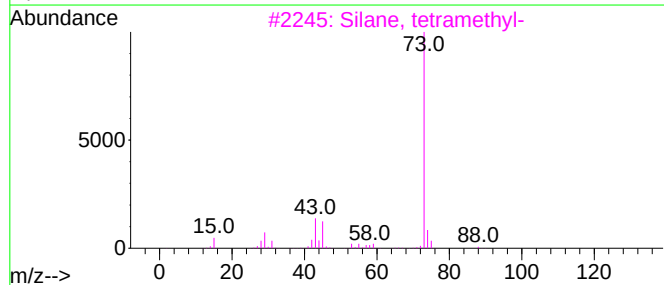
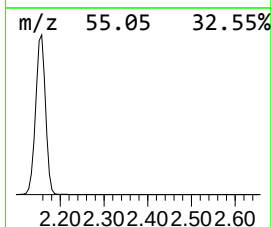
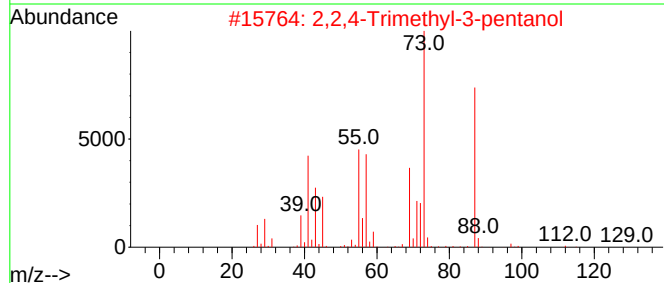
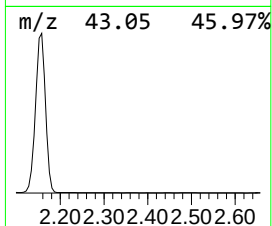
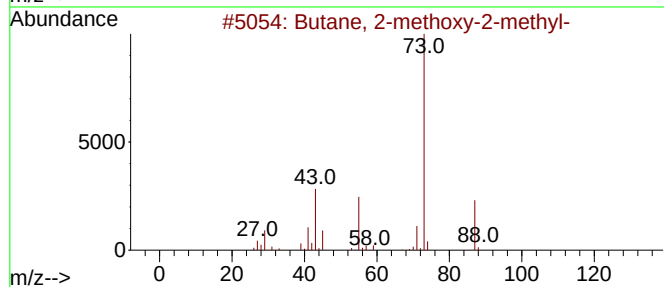
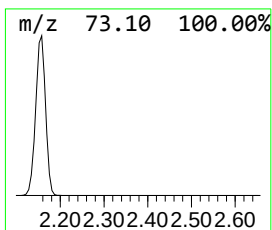
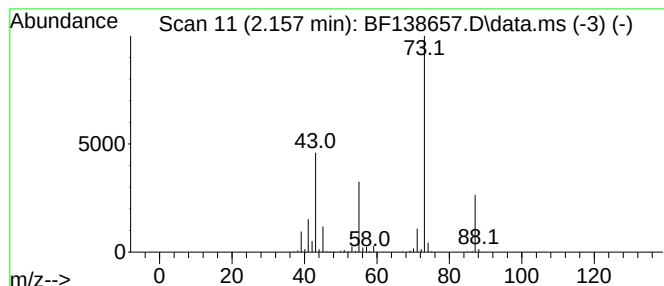
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.157	76.94 ng	1541250	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			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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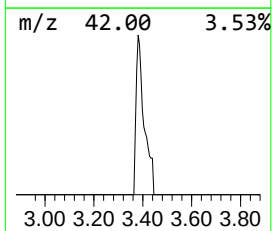
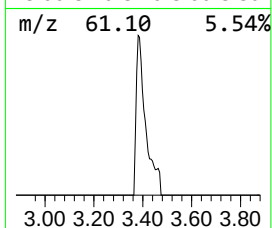
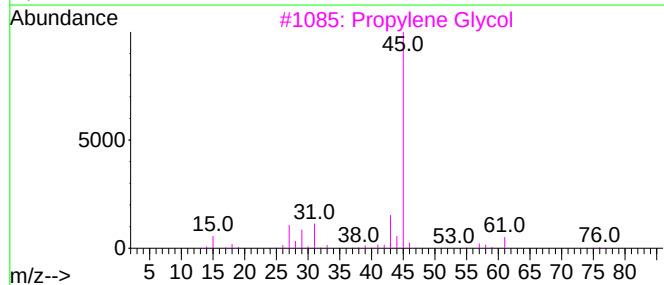
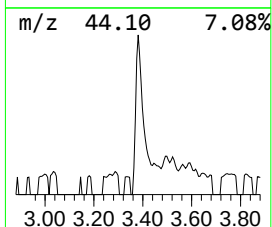
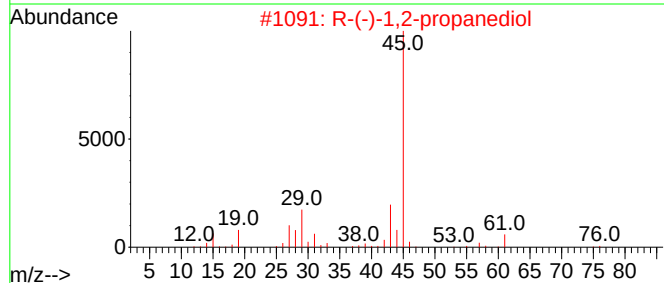
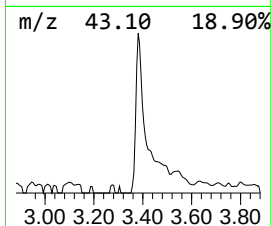
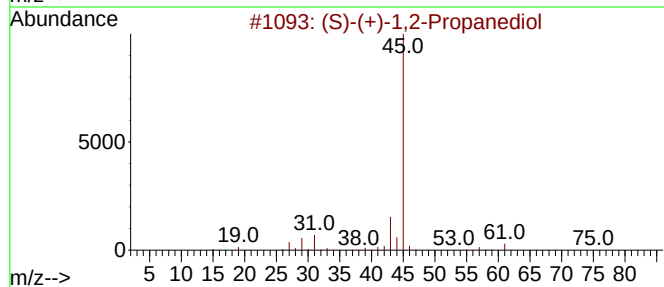
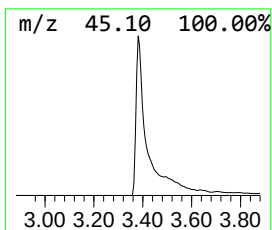
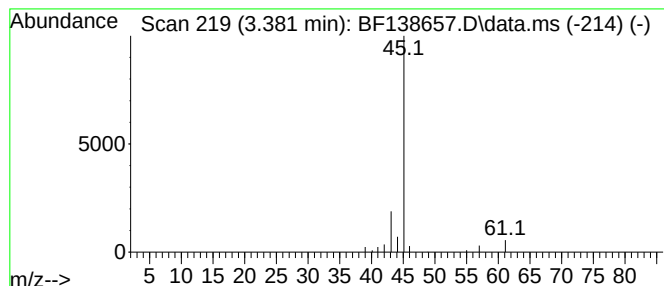
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Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.381	3.88 ng	77808	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	2-Butanol, (R)-			74	C4H10O	014898-79-4	9
5	Isopropyl Alcohol			60	C3H8O	000067-63-0	9



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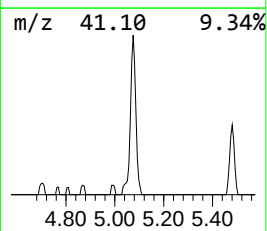
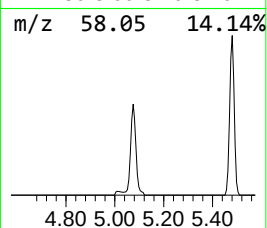
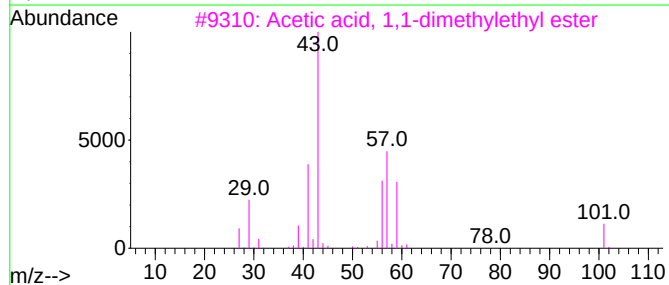
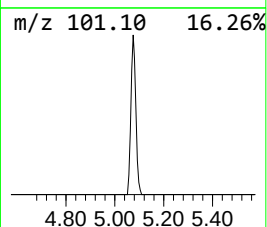
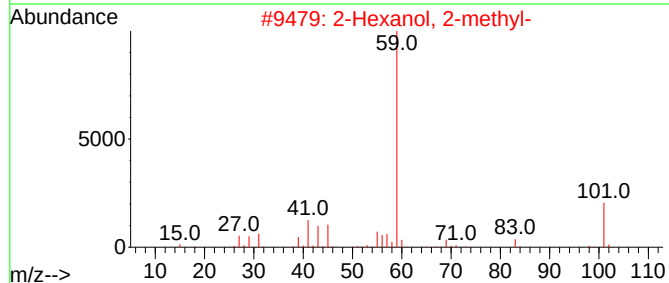
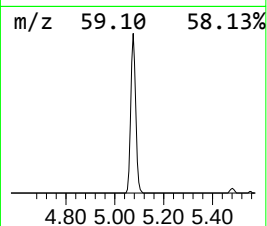
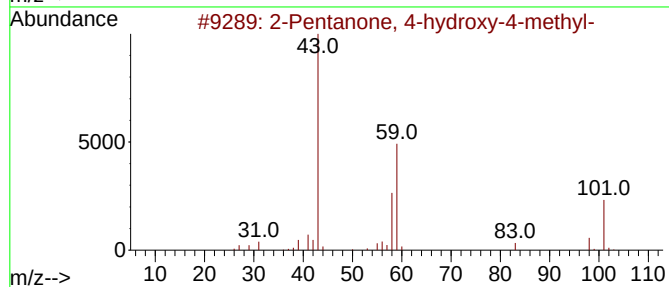
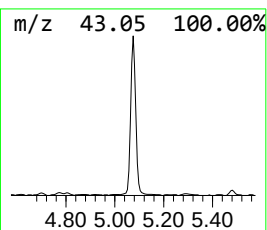
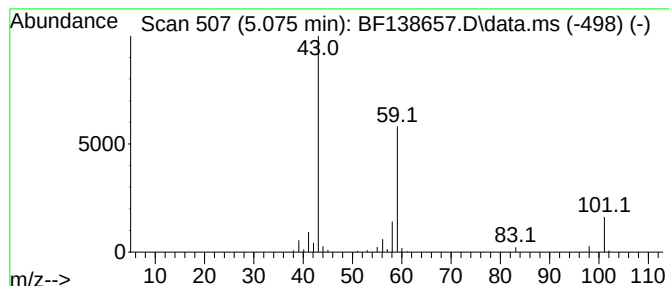
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	6.39 ng	128075	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			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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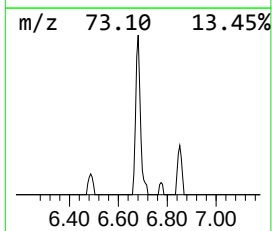
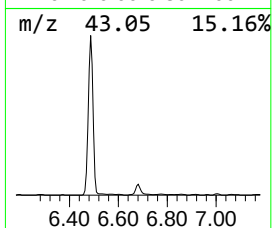
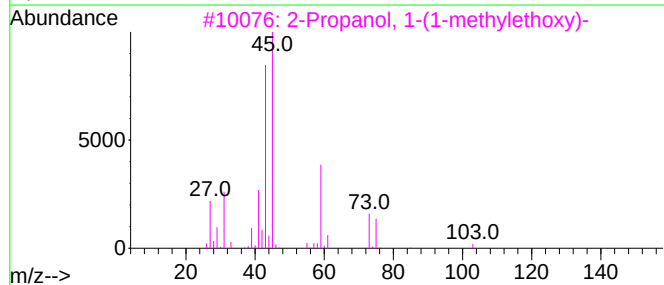
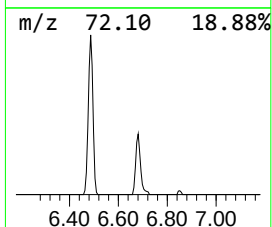
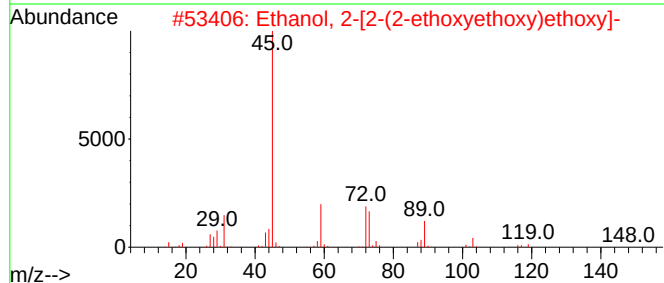
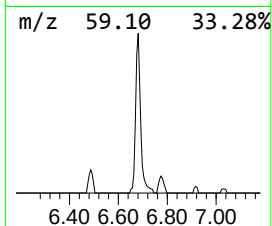
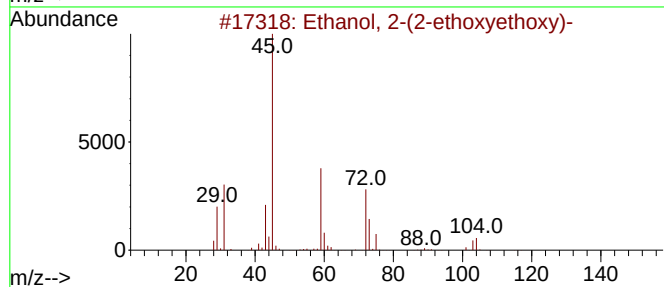
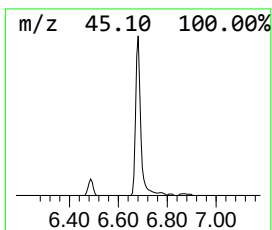
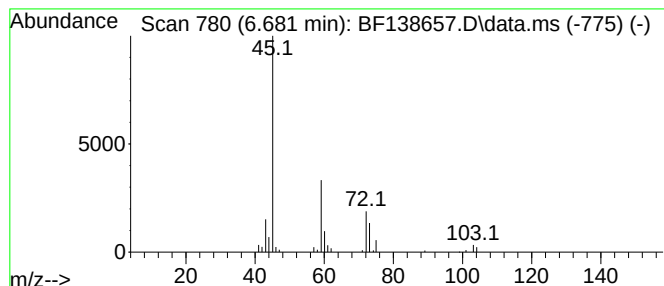
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Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.681	3.28 ng	65783	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-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	64
3			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	39
4			Ethyl ether	74	C4H10O	000060-29-7	38
5			Methoxyacetic acid, butyl ester	146	C7H14O3	017640-22-1	33



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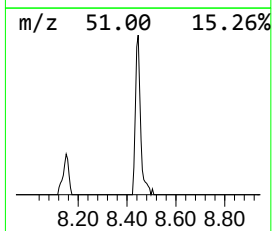
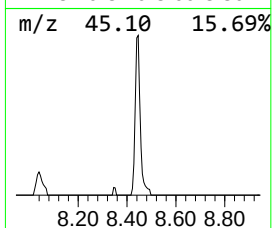
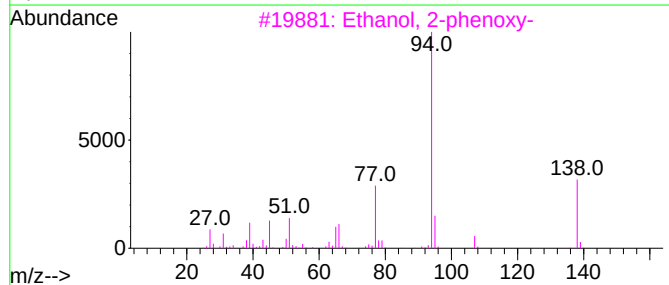
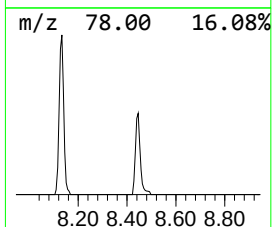
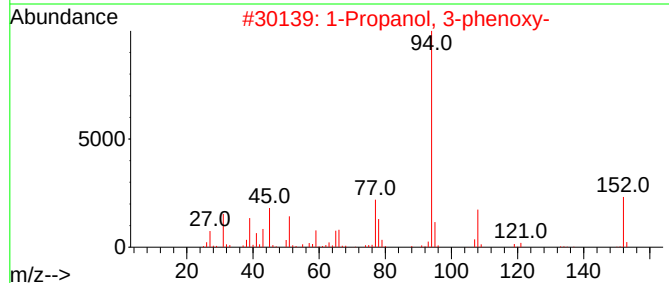
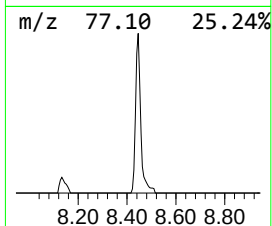
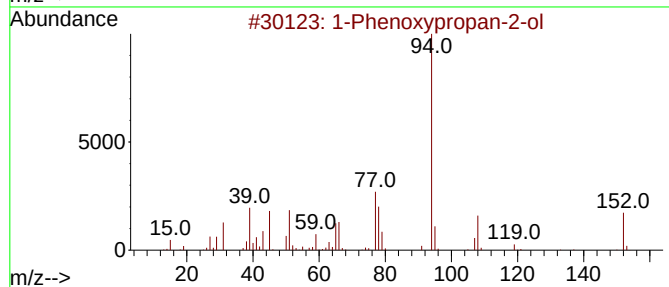
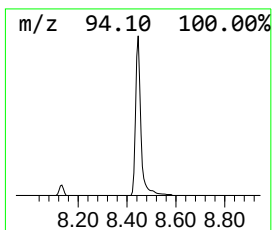
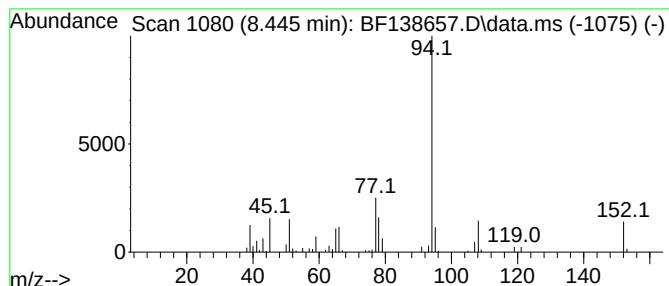
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Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.445	4.43 ng	126376	Naphthalene-d8	8.133

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	91
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			Benzene, (1-methylpropoxy)-	150	C10H14O	010574-17-1	53
5			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	53



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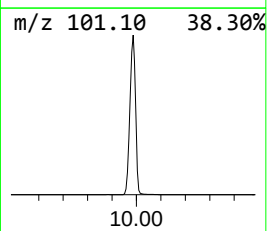
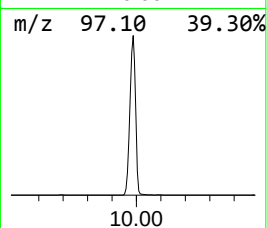
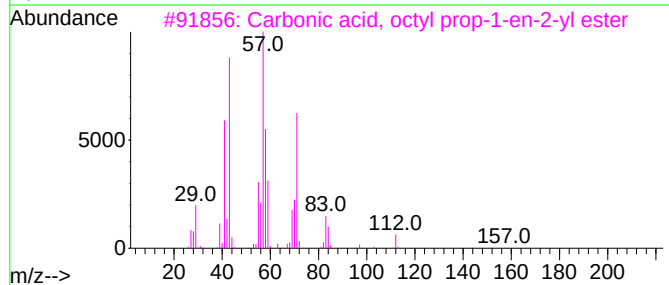
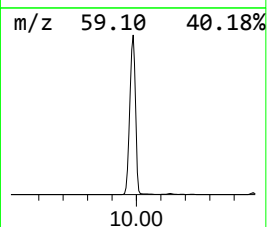
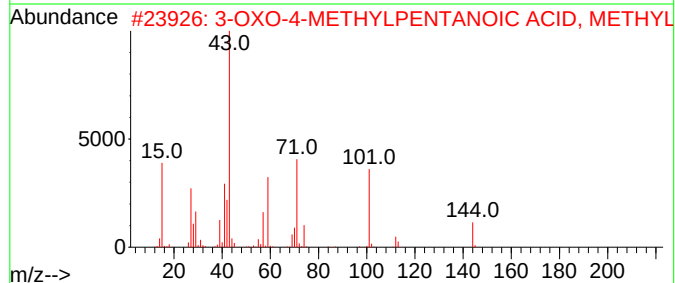
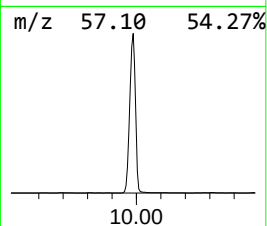
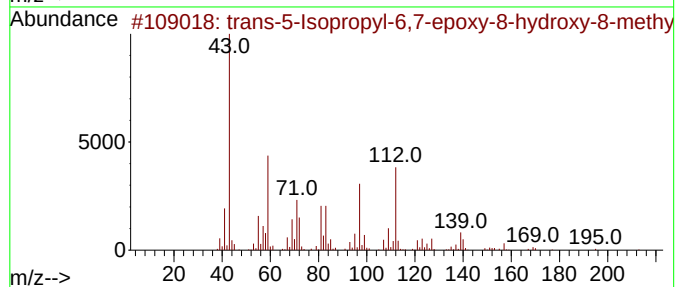
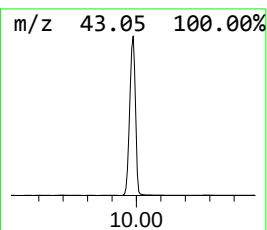
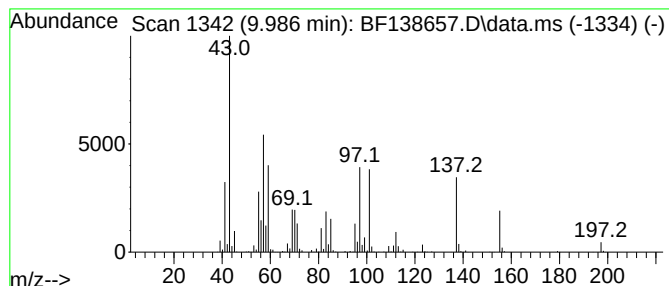
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown9.986 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.986	104.28 ng	3138560	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	25
2			3-OXO-4-METHYLPENTANOIC ACID, ME...	144	C7H12O3	042558-54-3	16
3			Carbonic acid, octyl prop-1-en-2...	214	C12H22O3	1000382-54-0	12
4			11-Tricosene	322	C23H46	052078-56-5	12
5			3-Octanol, 2,6-dimethyl-, acetate	200	C12H24O2	123232-57-5	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
Data File : BF138657.D
Acq On : 25 Jul 2024 17:20
Operator : RC/JU
Sample : P3357-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-854-J-SO-3-3.5-072024

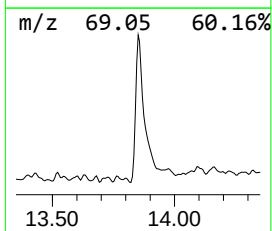
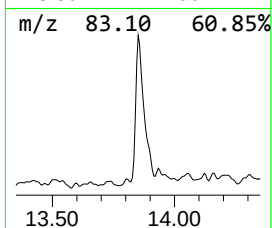
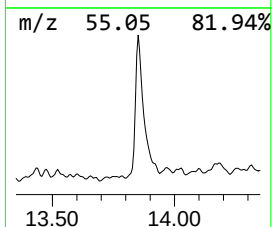
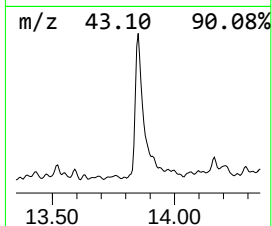
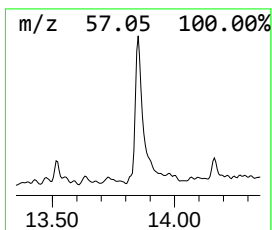
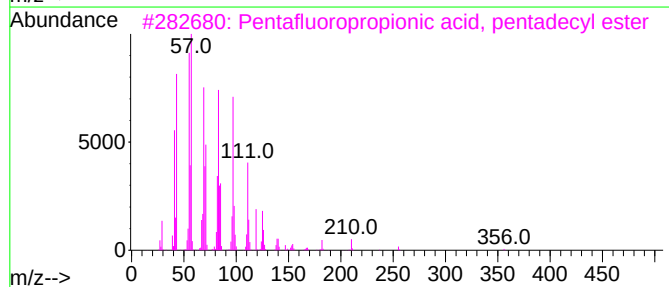
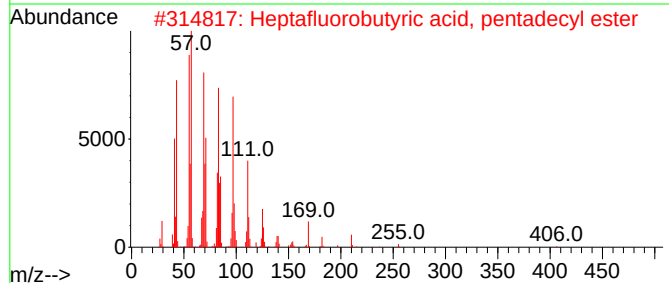
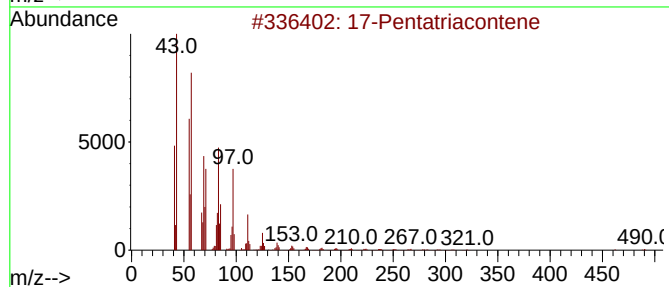
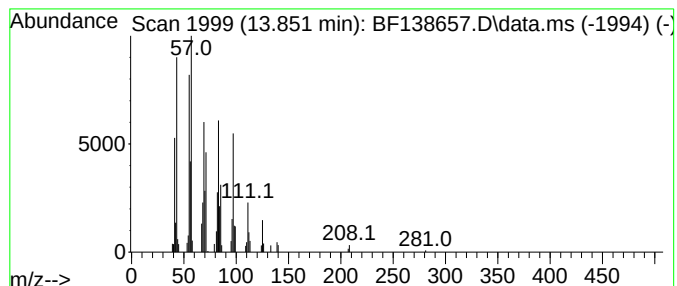
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 17-Pentatriacontene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	6.72 ng	107430	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	91
2			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
3			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
4			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
5			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
Data File : BF138657.D
Acq On : 25 Jul 2024 17:20
Operator : RC/JU
Sample : P3357-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-854-J-SO-3-3.5-072024

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...	2.157	76.9	ng	1541250	1	6.851	400628	20.0
(S)-(+)-1,2-Pro...	3.381	3.9	ng	77808	1	6.851	400628	20.0
2-Pentanone, 4-...	5.075	6.4	ng	128075	1	6.851	400628	20.0
Ethanol, 2-(2-e...	6.681	3.3	ng	65783	1	6.851	400628	20.0
1-Phenoxypropan...	8.445	4.4	ng	126376	2	8.133	570658	20.0
unknown9.986	9.986	104.3	ng	3138560	3	9.886	601954	20.0
17-Pentatriacon...	13.851	6.7	ng	107430	5	14.004	319682	20.0