

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
 Data File : BF138655.D
 Acq On : 25 Jul 2024 16:19
 Operator : RC/JU
 Sample : P3357-04
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-857-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: BF138655.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	9	20	rVB	819601	1283794	86.58%	11.022%
2	3.369	212	217	239	rBV	38042	97367	6.57%	0.836%
3	5.069	495	506	516	rBV	66227	96682	6.52%	0.830%
4	5.481	570	576	587	rBV	962404	1281514	86.43%	11.003%
5	6.487	741	747	760	rBV	1033752	1340242	90.39%	11.507%
6	6.681	773	780	793	rBV	25886	38026	2.56%	0.326%
7	6.851	804	809	814	rBV	336272	405615	27.36%	3.482%
8	7.410	898	904	914	rBV	631814	851582	57.43%	7.311%
9	7.669	944	948	953	rVB	12632	15840	1.07%	0.136%
10	8.133	1021	1027	1032	rBV	438531	545128	36.77%	4.680%
11	8.445	1075	1080	1095	rBV	62569	92305	6.23%	0.792%
12	9.204	1203	1209	1220	rBV	1151246	1482721	100.00%	12.730%
13	9.886	1320	1325	1335	rBV	486028	607465	40.97%	5.215%
14	9.980	1335	1341	1348	rVB	51517	80077	5.40%	0.688%
15	10.674	1454	1459	1474	rBV	674307	883559	59.59%	7.586%
16	11.369	1572	1577	1587	rBV	450363	583831	39.38%	5.013%
17	11.898	1661	1667	1676	rBV3	16105	30478	2.06%	0.262%
18	12.951	1841	1846	1851	rBV	874034	1099948	74.18%	9.444%
19	13.851	1991	1999	2018	rBV2	45644	112587	7.59%	0.967%
20	14.010	2021	2026	2035	rVB	236087	317280	21.40%	2.724%
21	14.468	2099	2104	2108	rBV	24482	37991	2.56%	0.326%
22	15.109	2209	2213	2217	rVB	13059	18230	1.23%	0.157%
23	15.192	2224	2227	2233	rVB3	12073	17979	1.21%	0.154%
24	15.468	2268	2274	2285	rVB	202895	327146	22.06%	2.809%

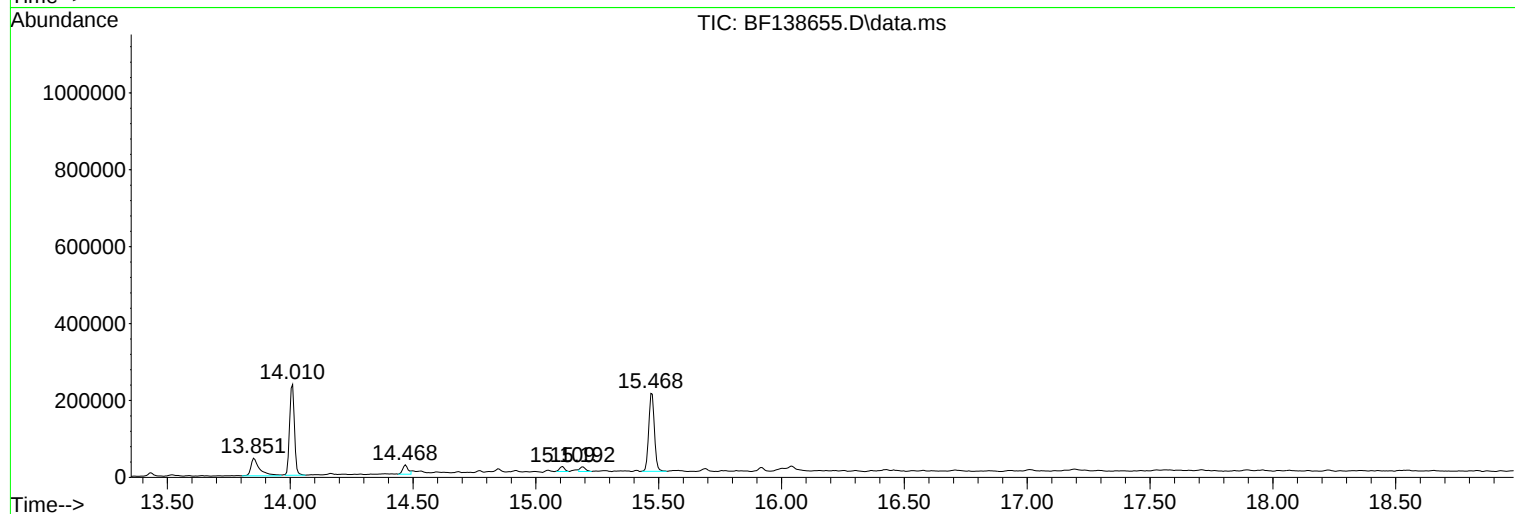
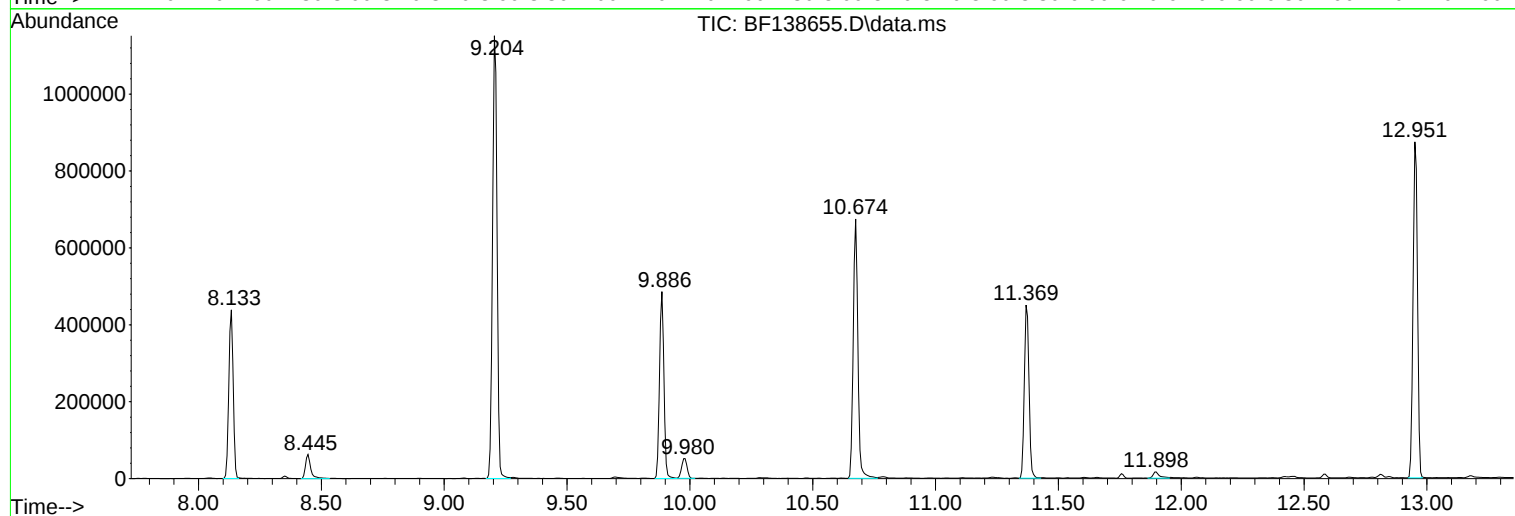
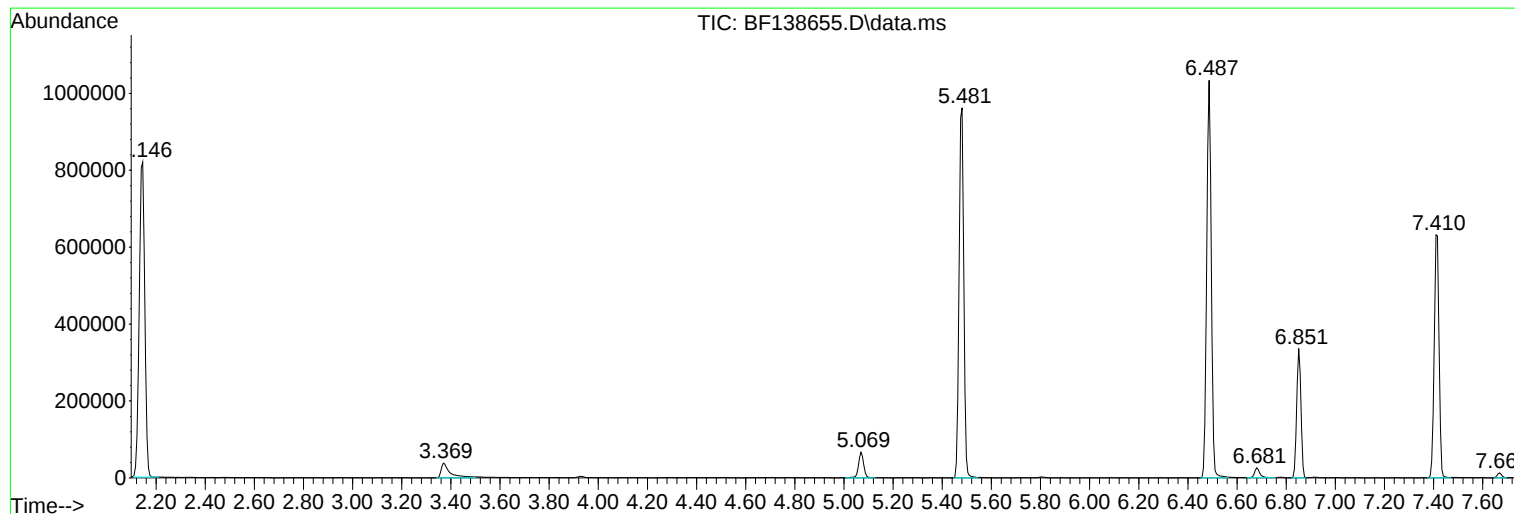
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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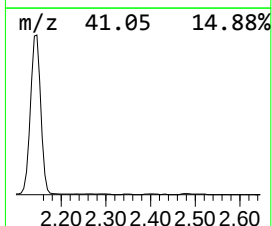
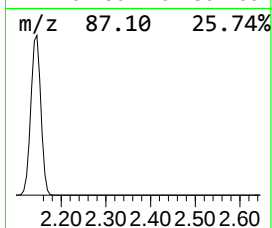
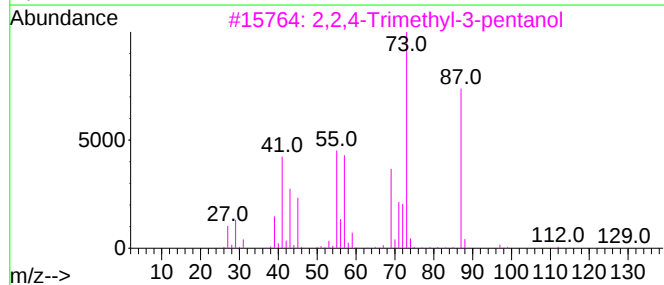
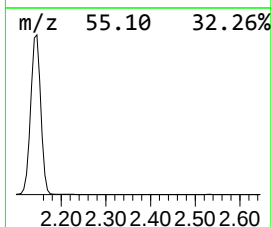
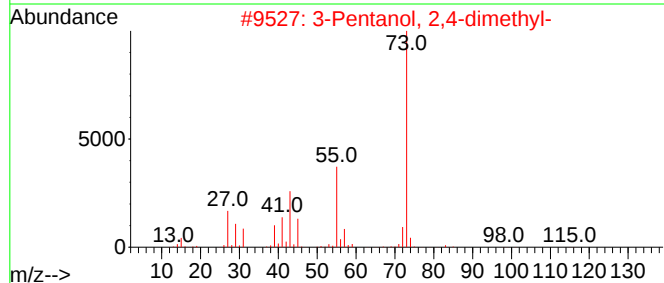
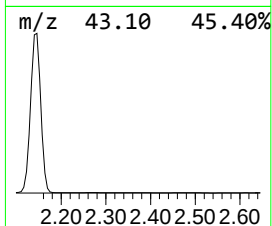
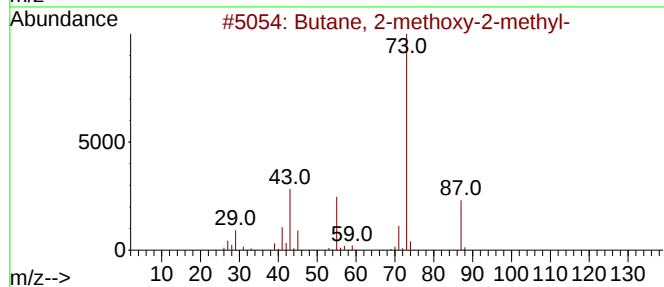
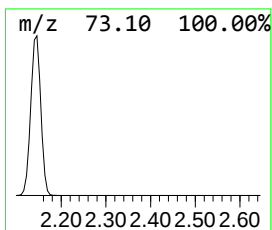
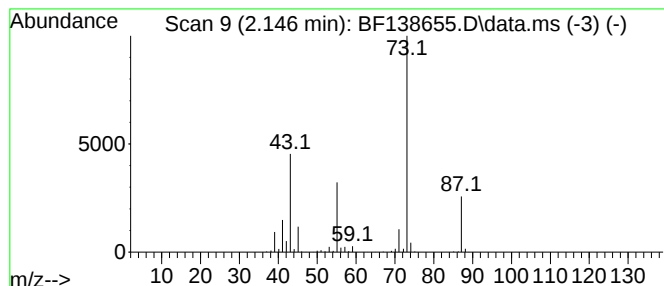
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	63.30 ng	1283790	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			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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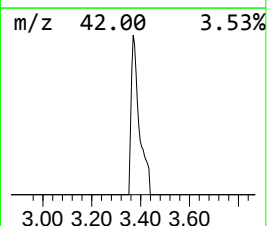
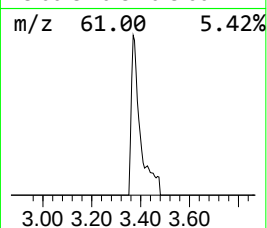
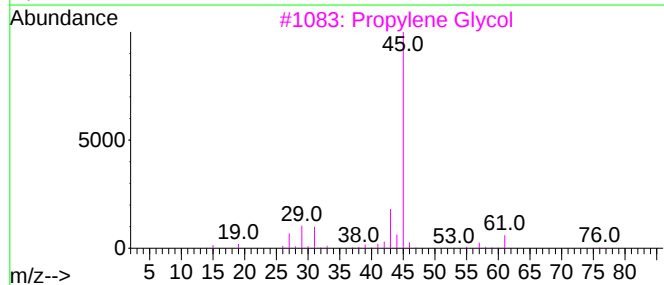
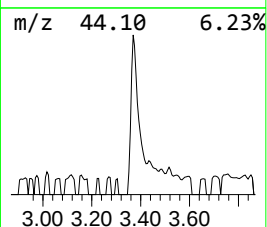
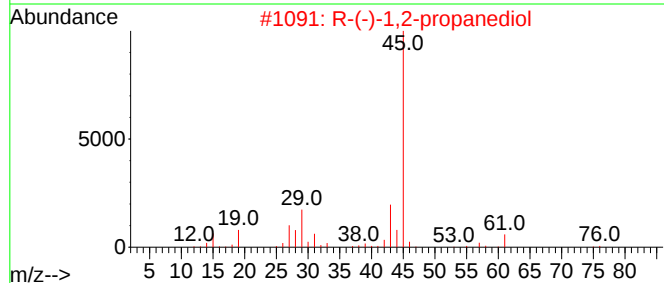
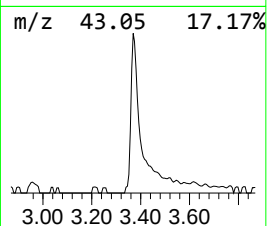
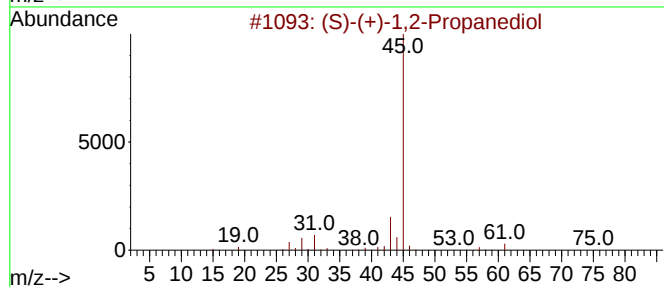
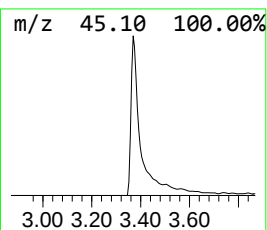
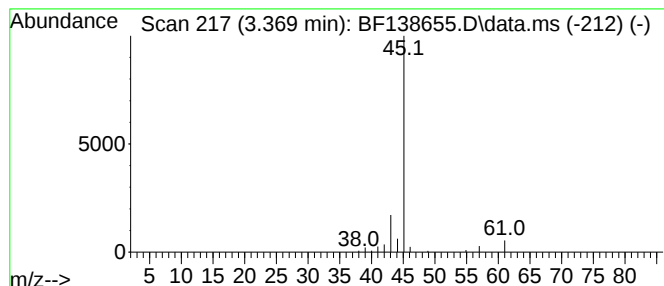
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Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.369	4.80 ng	97367	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	Isopropyl Alcohol			60	C3H8O	000067-63-0	9
5	Formamide			45	CH3NO	000075-12-7	7



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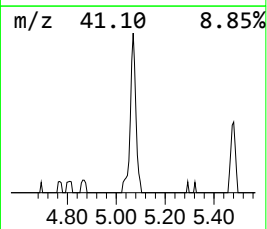
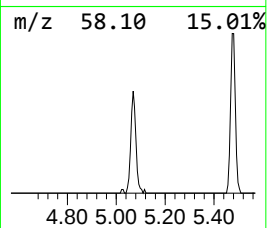
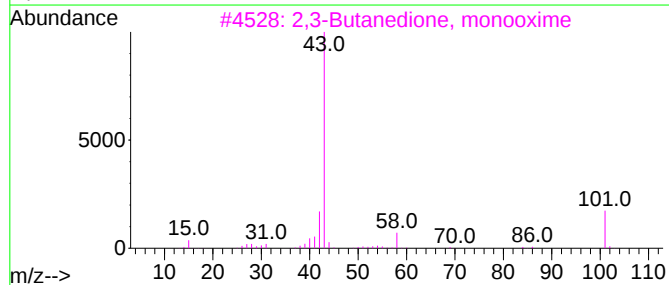
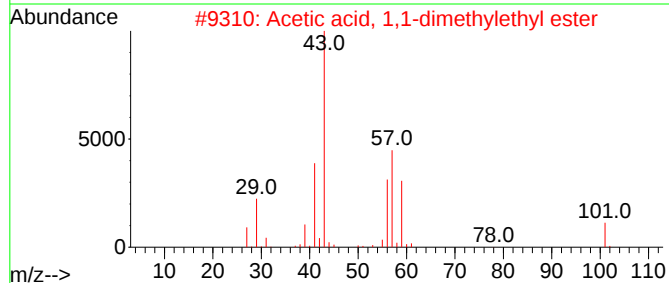
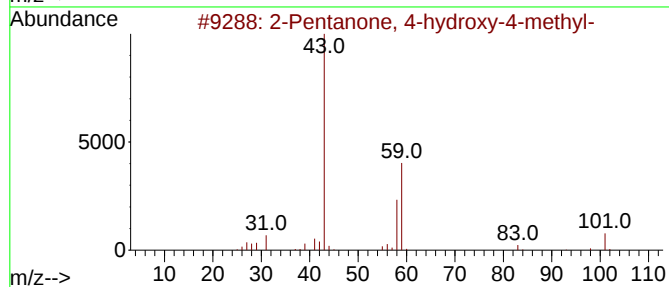
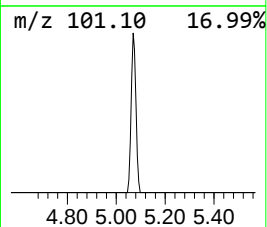
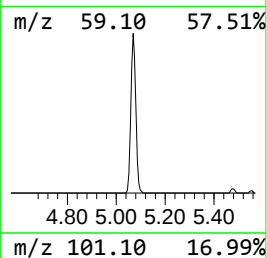
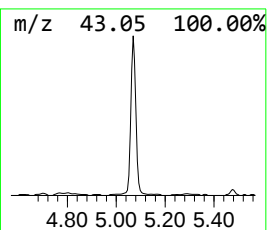
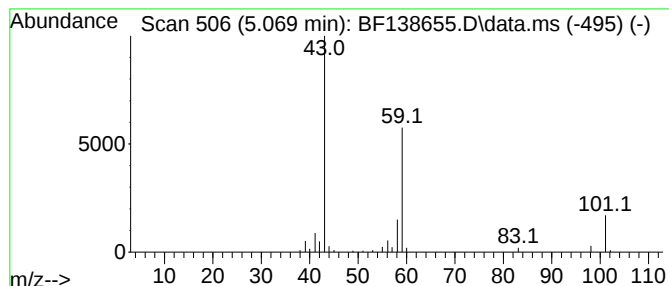
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	4.77 ng	96682	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	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		



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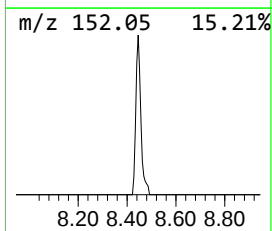
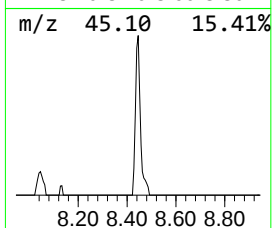
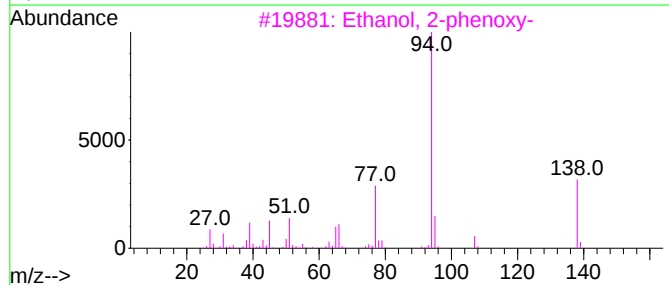
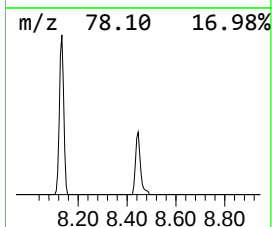
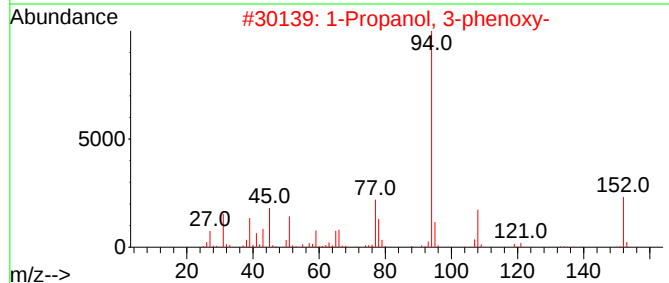
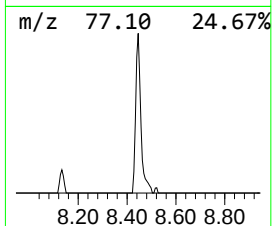
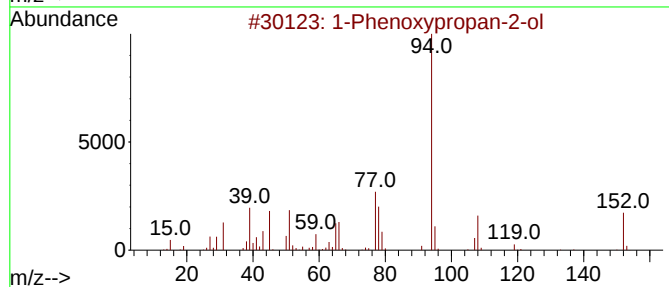
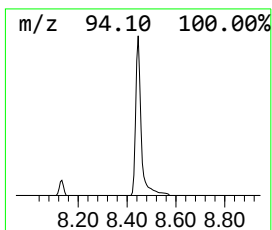
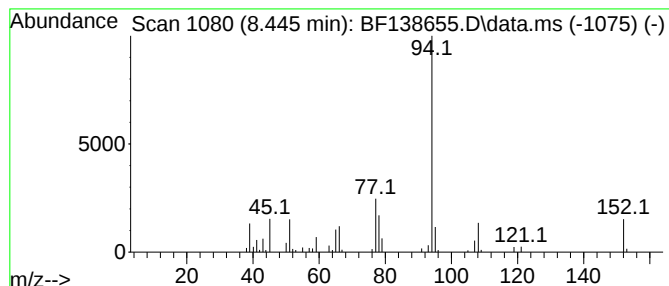
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Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.445	3.39 ng	92305	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	87
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
5			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59



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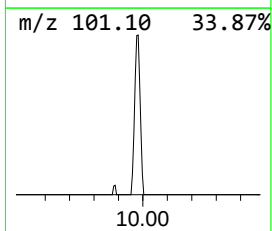
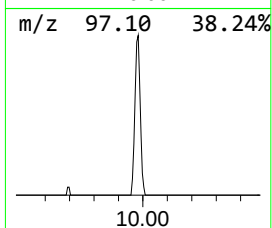
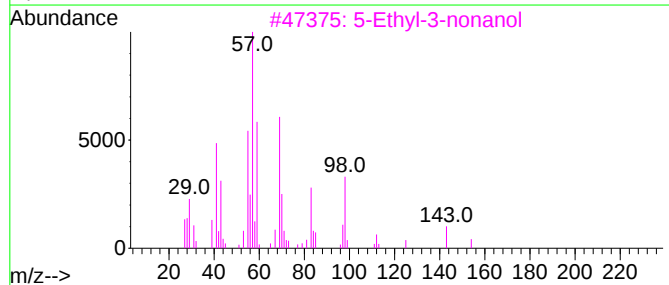
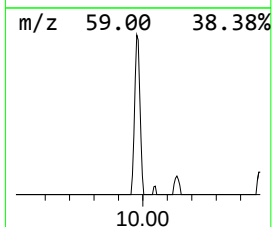
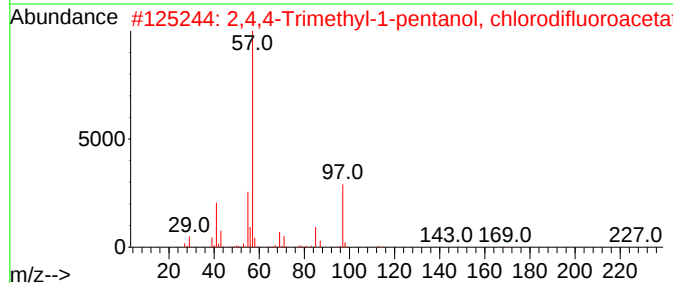
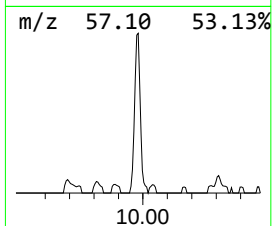
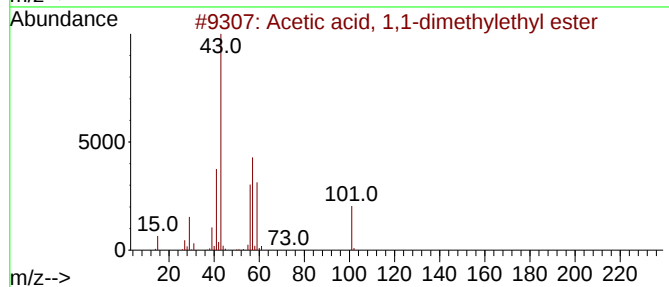
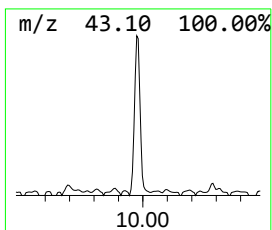
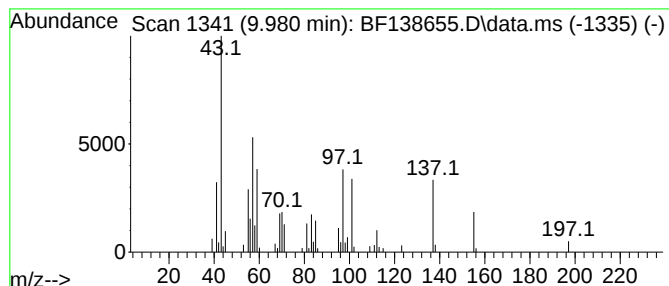
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Peak Number 5 unknown9.980 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.980	2.64 ng	80077	Acenaphthene-d10	9.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	22
2			2,4,4-Trimethyl-1-pentanol, chlo...	242	C10H17ClF2O2	1000447-27-2	14
3			5-Ethyl-3-nonanol	172	C11H24O	019780-71-3	14
4			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	12
5			3-Tetradecanol acetate	256	C16H32O2	051354-23-5	12



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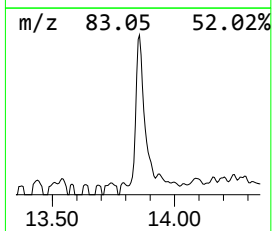
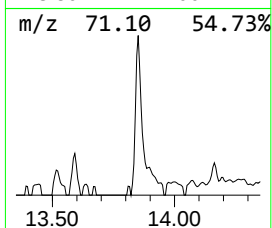
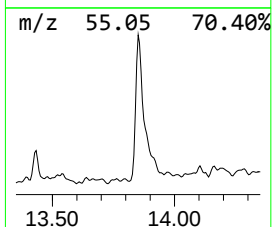
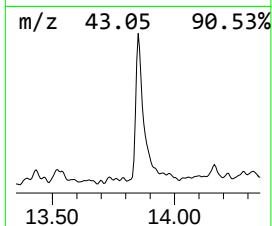
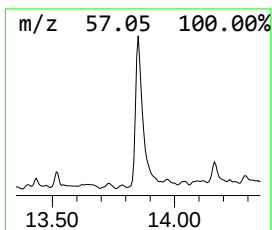
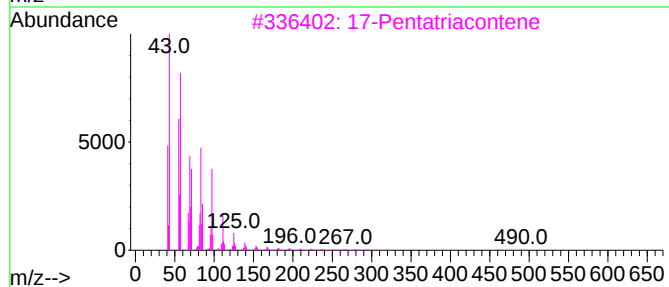
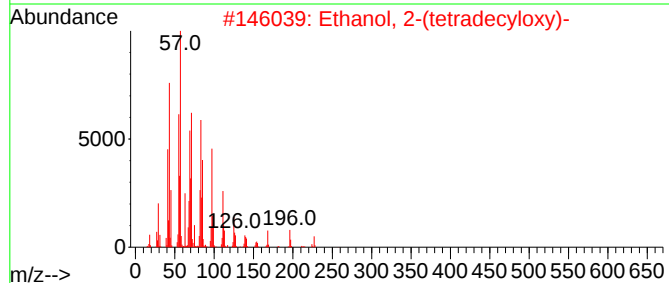
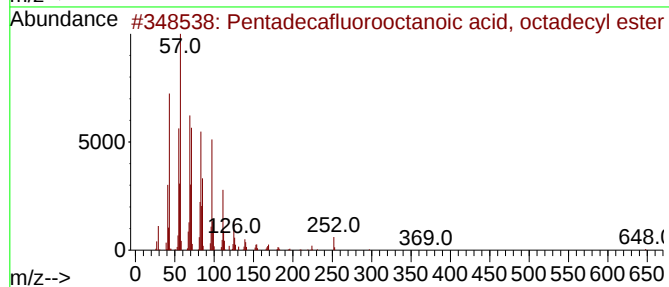
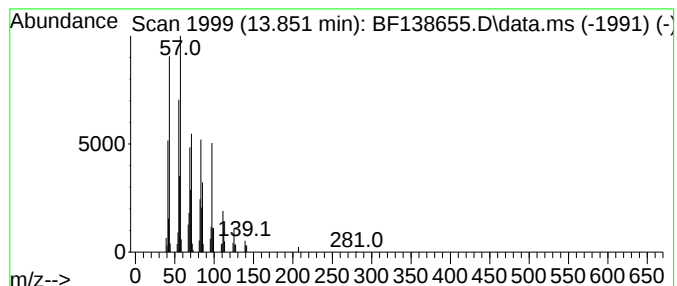
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentadecafluorooctanoic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	7.10 ng	112587	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
3			17-Pentatriacontene	491	C35H70	006971-40-0	90
4			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	87
5			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
Data File : BF138655.D
Acq On : 25 Jul 2024 16:19
Operator : RC/JU
Sample : P3357-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-857-J-SO-3-3.5-072024

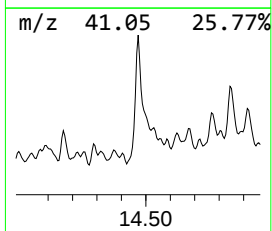
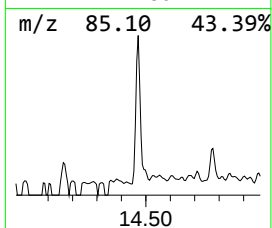
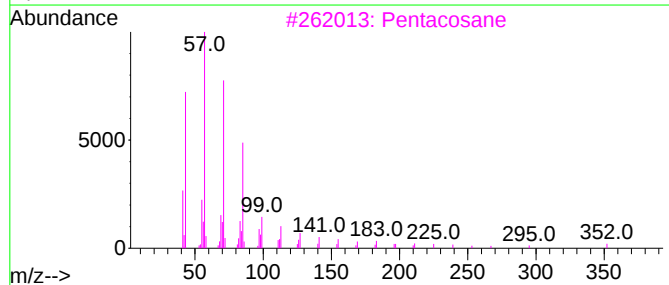
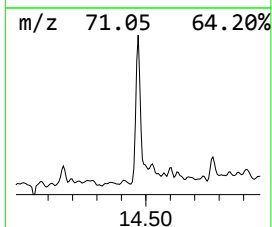
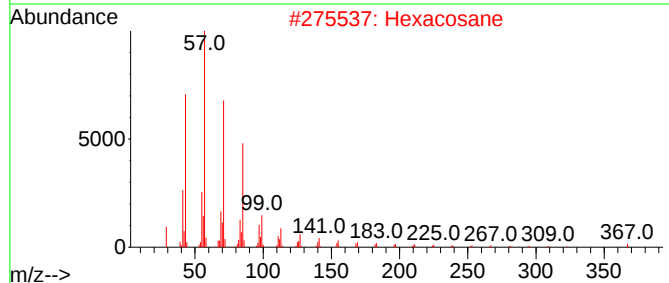
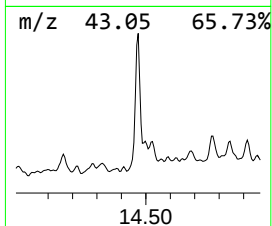
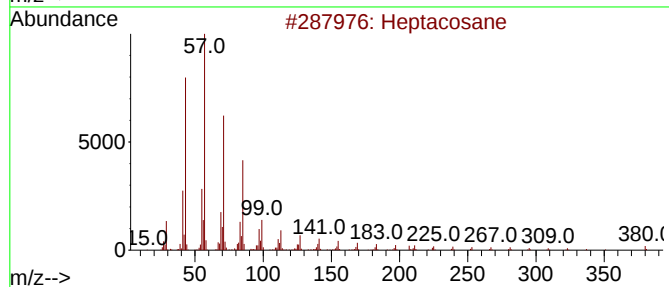
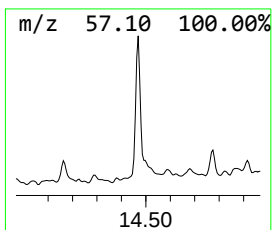
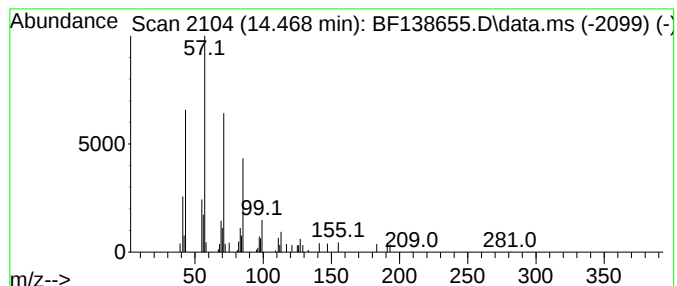
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.468	2.39 ng	37991	Chrysene-d12	14.010

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptacosane	380	C27H56	000593-49-7	87
2		Hexacosane	366	C26H54	000630-01-3	87
3		Pentacosane	352	C25H52	000629-99-2	87
4		Octadecane	254	C18H38	000593-45-3	86
5		Tetracosane	338	C24H50	000646-31-1	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
Data File : BF138655.D
Acq On : 25 Jul 2024 16:19
Operator : RC/JU
Sample : P3357-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-857-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\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.146	63.3	ng	1283790	1	6.851	405615	20.0
(S)-(+)-1,2-Pro...	3.369	4.8	ng	97367	1	6.851	405615	20.0
2-Pentanone, 4-...	5.069	4.8	ng	96682	1	6.851	405615	20.0
1-Phenoxypropan...	8.445	3.4	ng	92305	2	8.133	545128	20.0
unknown9.980	9.980	2.6	ng	80077	3	9.886	607465	20.0
Pentadecafluoro...	13.851	7.1	ng	112587	5	14.010	317280	20.0
Heptacosane	14.468	2.4	ng	37991	5	14.010	317280	20.0