

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092624\
 Data File : BF139562.D
 Acq On : 26 Sep 2024 22:50
 Operator : RC/JU
 Sample : P4198-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP2-WC-1

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-BF091324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139562.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.158	4	11	26	rVB	1386698	2110110	100.00%	15.622%
2	3.375	212	218	245	rBV	27304	83668	3.97%	0.619%
3	5.087	499	509	517	rBV	74409	113427	5.38%	0.840%
4	5.493	572	578	583	rBV	1113079	1424478	67.51%	10.546%
5	6.504	744	750	767	rVB	1145572	1498773	71.03%	11.096%
6	6.698	777	783	794	rBV	25193	37799	1.79%	0.280%
7	6.875	808	813	818	rBV	334177	395957	18.76%	2.931%
8	7.434	902	908	913	rBV	731954	939646	44.53%	6.956%
9	8.157	1026	1031	1044	rVB	410851	517947	24.55%	3.835%
10	8.469	1079	1084	1094	rBV	43990	63523	3.01%	0.470%
11	9.228	1208	1213	1222	rBV	1244279	1612539	76.42%	11.938%
12	9.616	1276	1279	1283	rBV3	18159	26332	1.25%	0.195%
13	9.775	1302	1306	1309	rBV2	37261	56844	2.69%	0.421%
14	9.822	1310	1314	1317	rVB	46773	67376	3.19%	0.499%
15	9.910	1323	1329	1333	rBV	460190	592273	28.07%	4.385%
16	10.316	1395	1398	1402	rBV2	77522	97608	4.63%	0.723%
17	10.698	1459	1463	1468	rBV	724933	952067	45.12%	7.048%
18	11.398	1578	1582	1591	rBV	471224	591624	28.04%	4.380%
19	12.980	1846	1851	1860	rVB	1199064	1529436	72.48%	11.323%
20	14.033	2025	2030	2045	rVB	313087	427200	20.25%	3.163%
21	15.510	2275	2281	2294	rBV	225485	368863	17.48%	2.731%

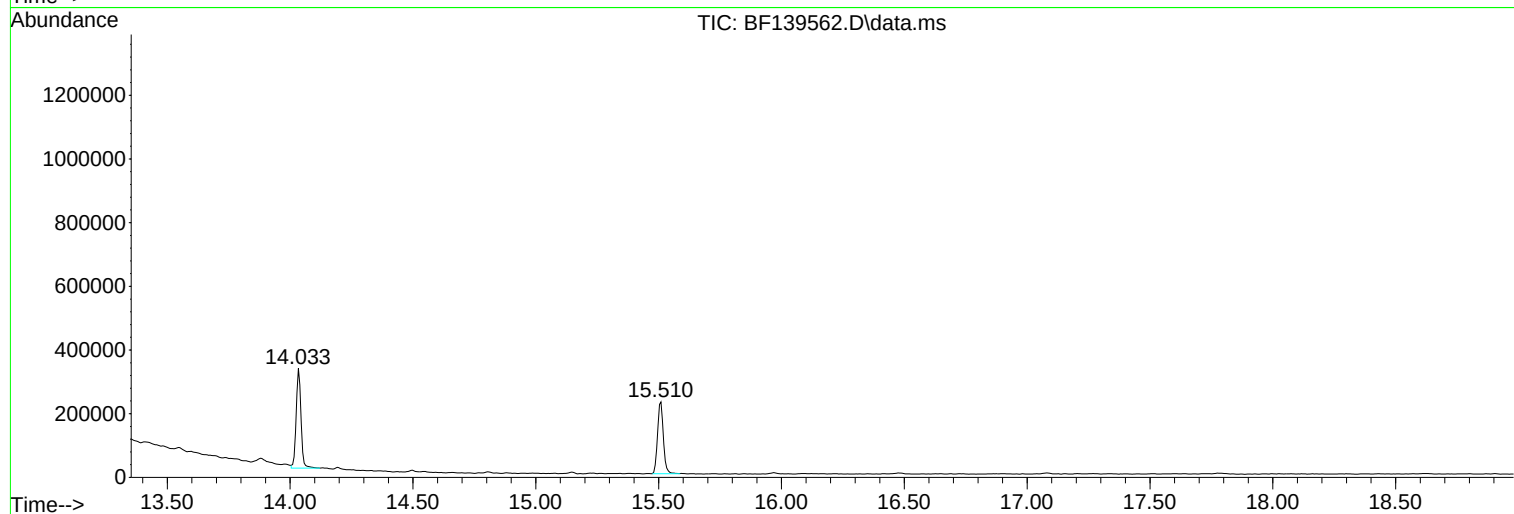
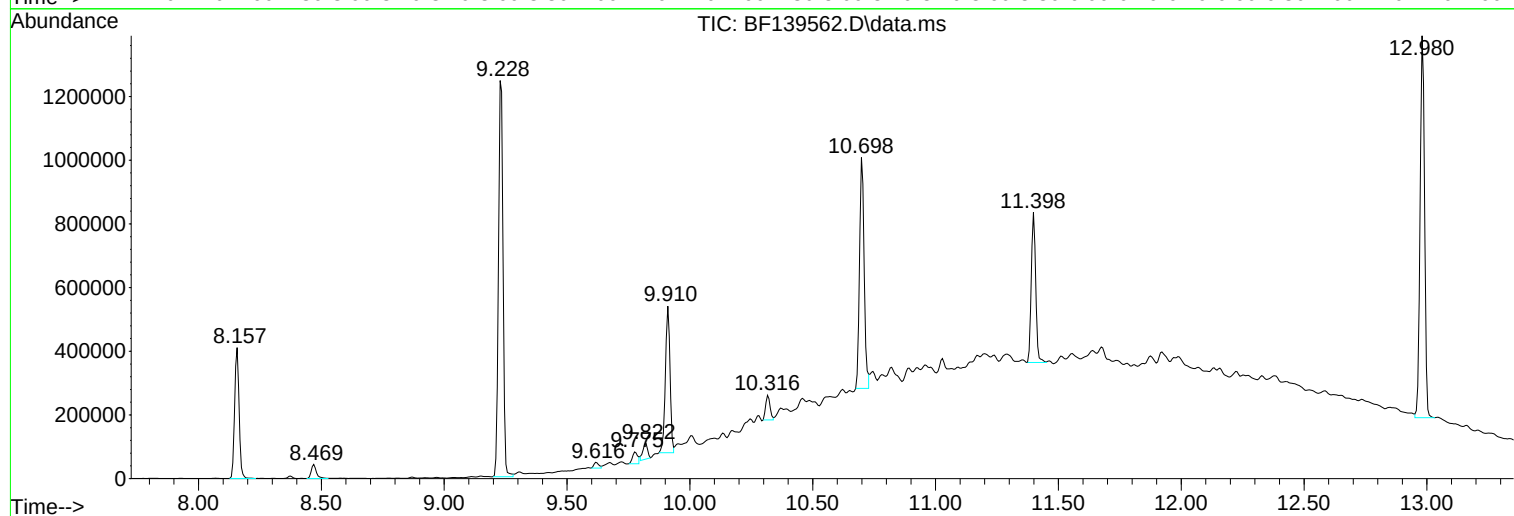
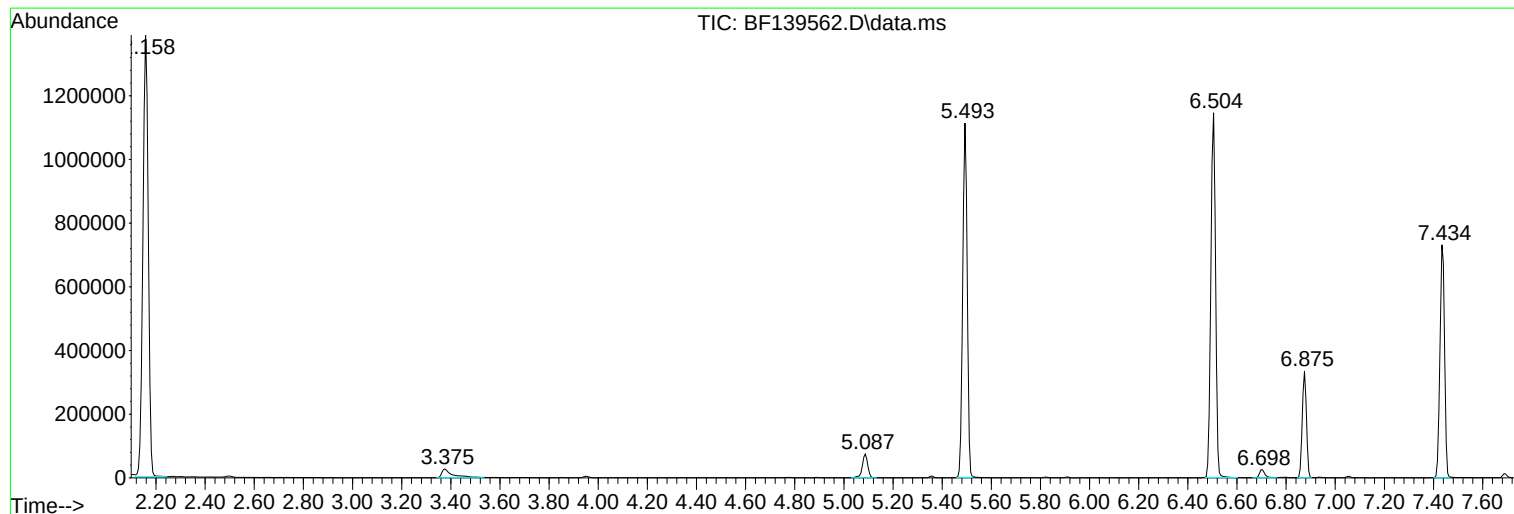
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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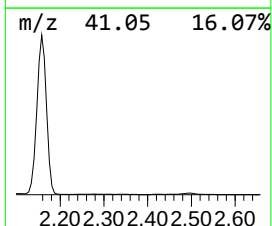
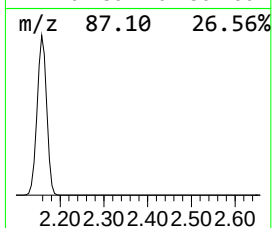
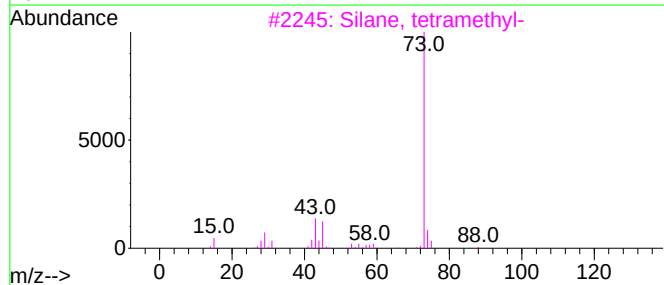
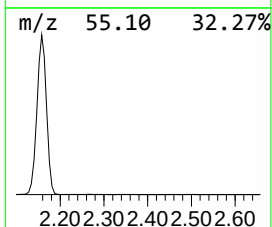
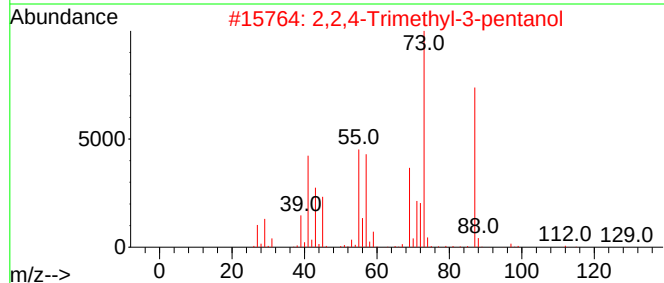
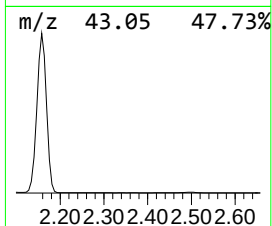
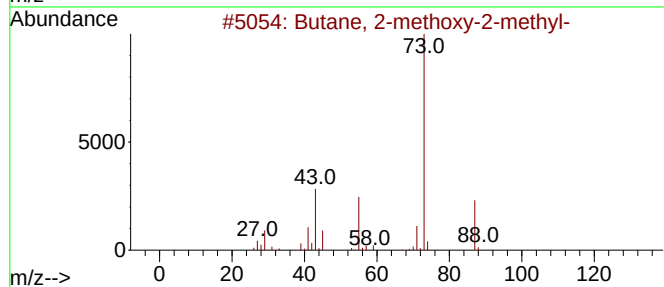
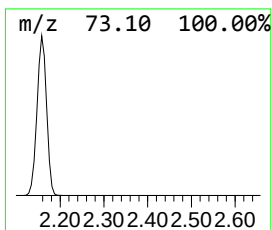
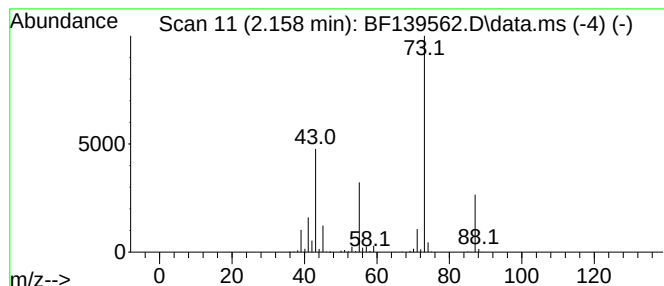
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.158	106.58 ng	2110110	1,4-Dichlorobenzene-d4	6.875

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			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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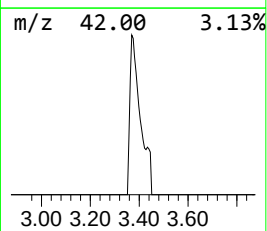
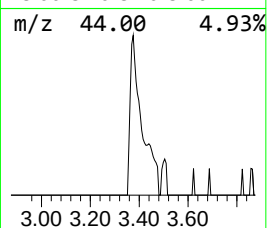
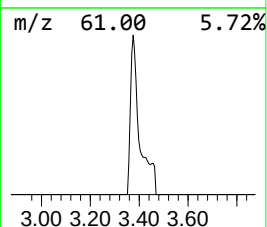
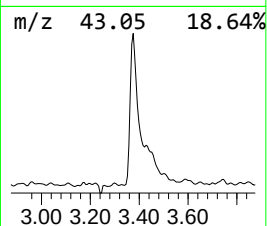
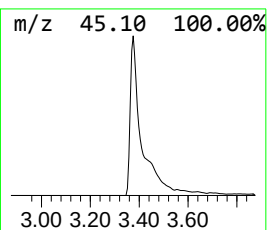
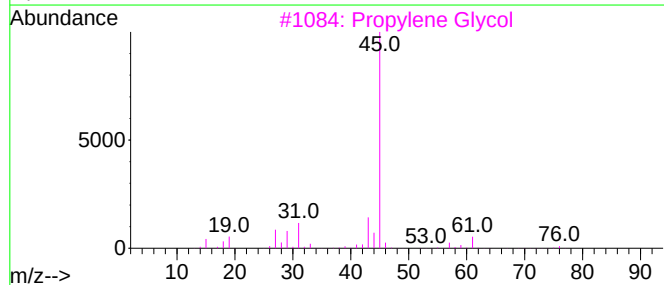
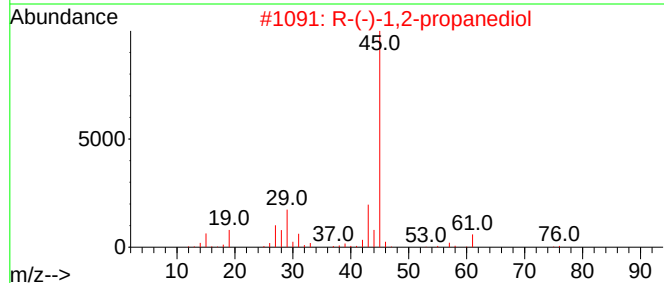
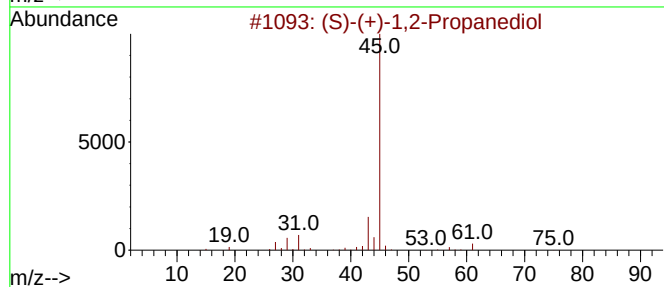
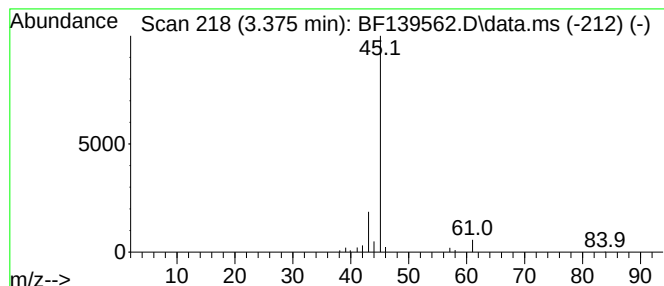
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown3.375 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.375	4.23 ng	83668	1,4-Dichlorobenzene-d4	6.875

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



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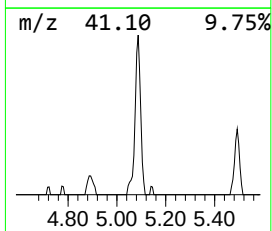
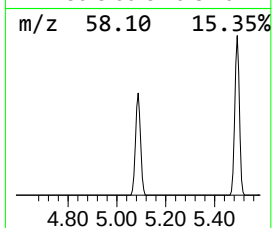
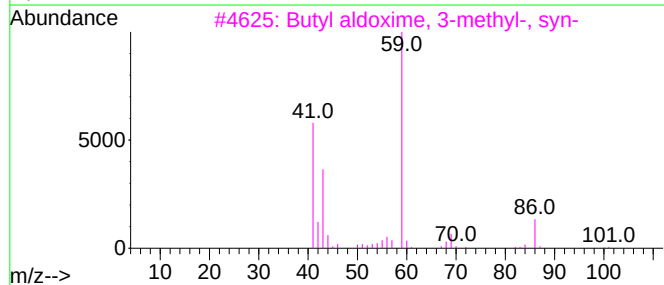
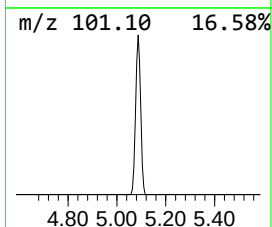
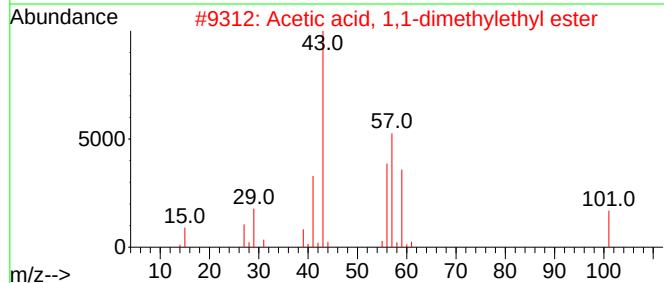
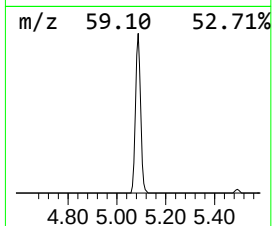
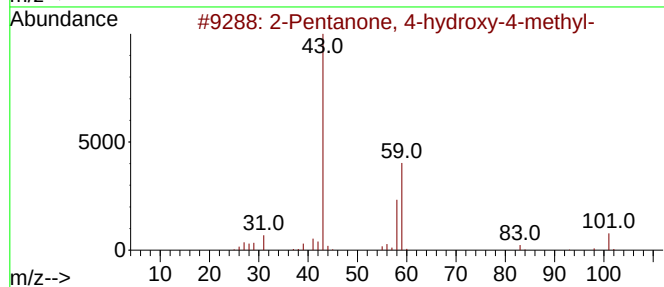
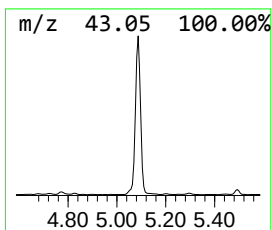
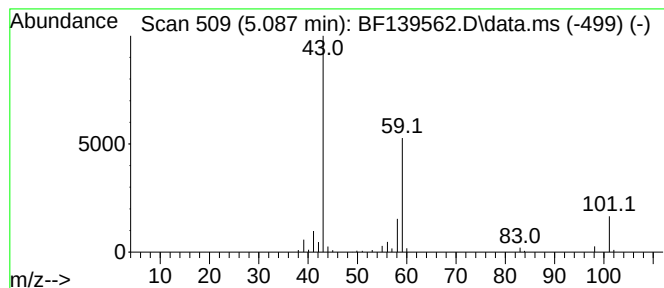
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	5.73 ng	113427	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38		
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23		
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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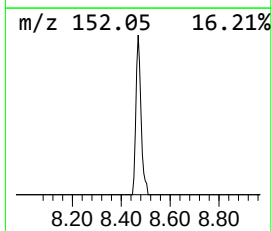
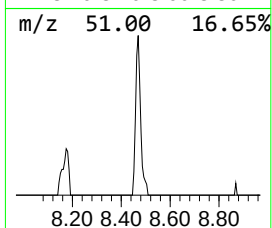
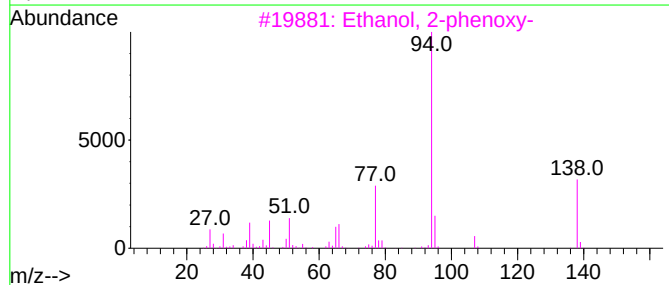
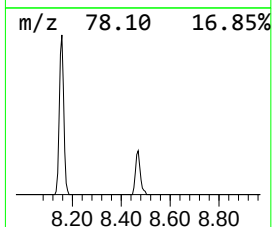
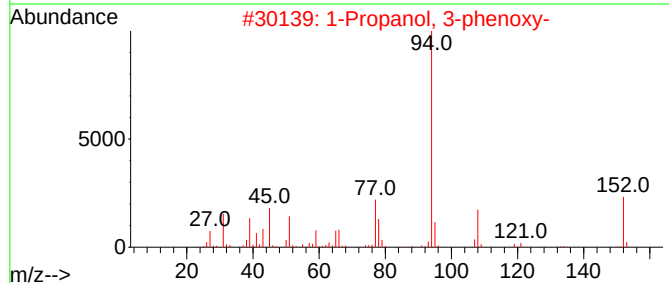
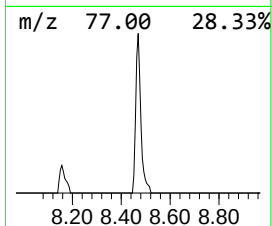
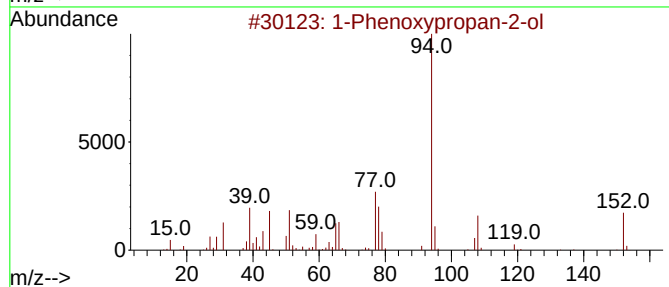
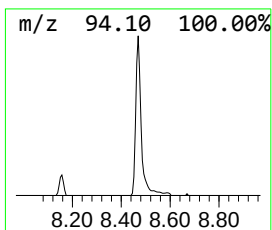
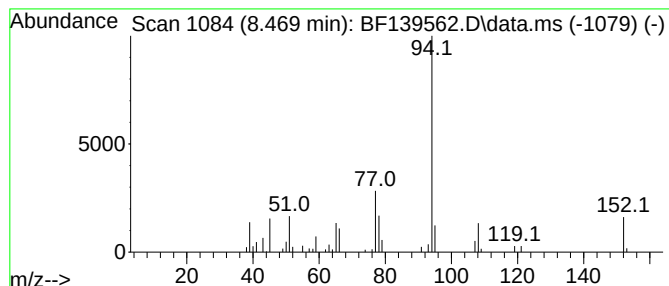
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Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.469	2.45 ng	63523	Naphthalene-d8	8.157

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		2-Hexen-4-yne, 2-methyl-	94	C7H10	058275-93-7	53
5		Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	53



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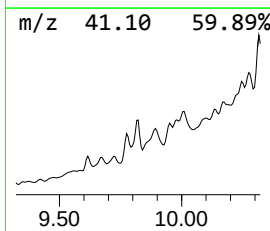
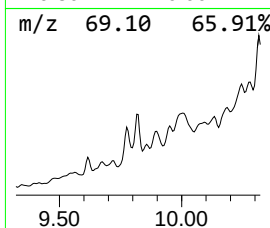
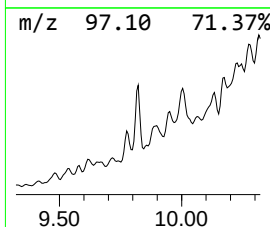
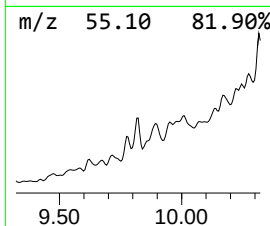
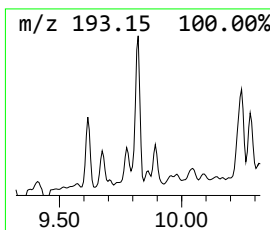
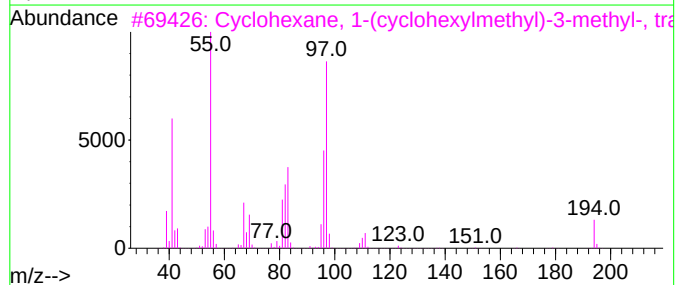
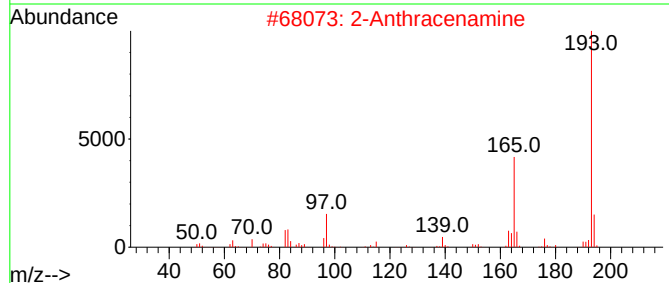
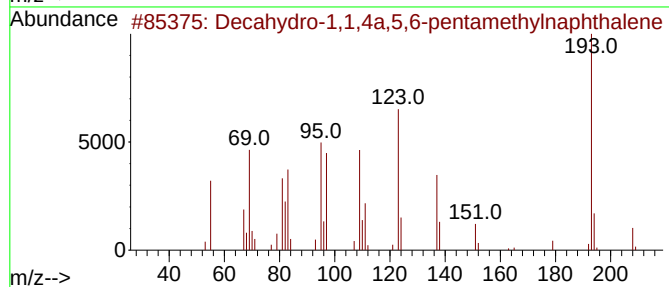
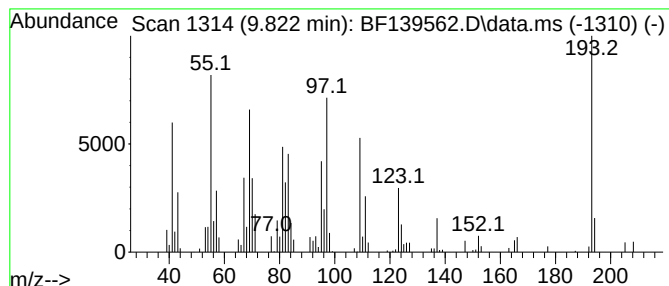
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown9.822 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.822	2.28 ng	67376	Acenaphthene-d10	9.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	43
2			2-Anthracenamine	193	C14H11N	000613-13-8	41
3			Cyclohexane, 1-(cyclohexylmethyl)...	194	C14H26	054823-95-9	30
4			4-Cyano-4'-methylbiphenyl	193	C14H11N	050670-50-3	25
5			Cyclohexane, 1-(cyclohexylmethyl)...	194	C14H26	054823-98-2	20



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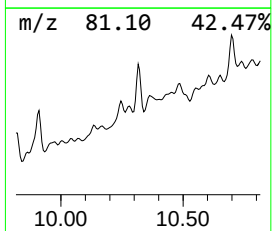
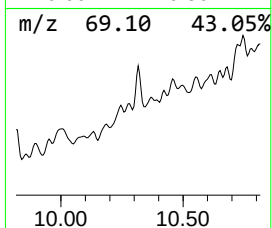
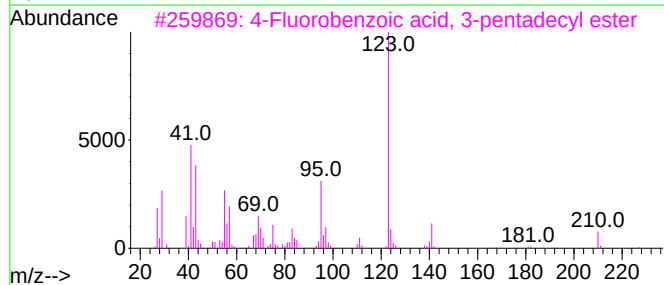
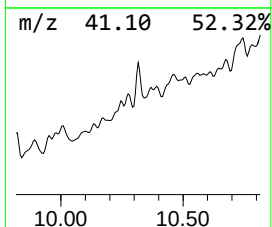
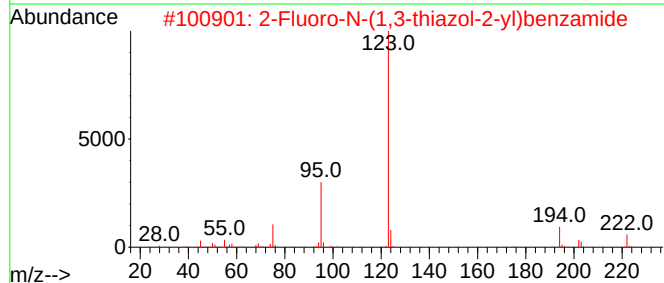
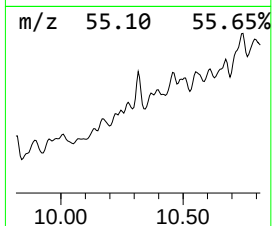
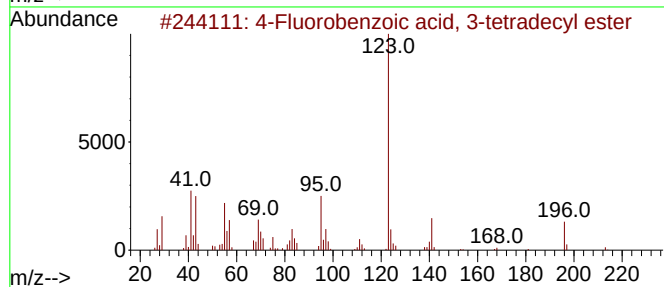
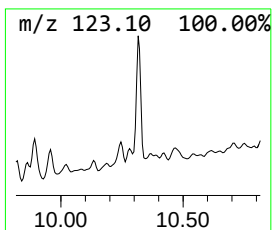
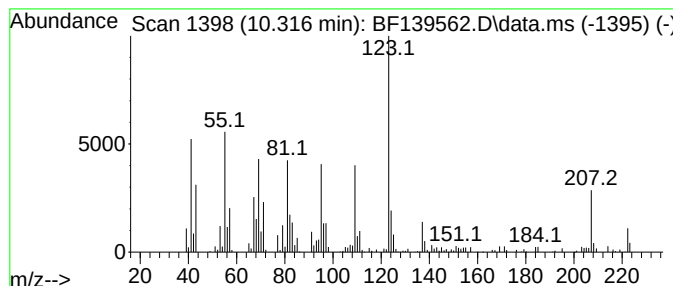
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown10.316 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.316	3.30 ng	97608	Acenaphthene-d10	9.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Fluorobenzoic acid, 3-tetradec...	336	C21H33FO2	1010280-68-1	47
2			2-Fluoro-N-(1,3-thiazol-2-yl)ben...	222	C10H7FN2OS	000319-38-0	43
3			4-Fluorobenzoic acid, 3-pentadec...	350	C22H35FO2	1000280-68-4	43
4			1-(1-Ethyl-2,3-dimethyl-cyclopen...	166	C11H18O	1000185-18-6	38
5			2-Pyrimidinamine, 4,6-dimethyl-	123	C6H9N3	000767-15-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092624\
Data File : BF139562.D
Acq On : 26 Sep 2024 22:50
Operator : RC/JU
Sample : P4198-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP2-WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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...	2.158	106.6	ng	2110110	1	6.875	395957	20.0
unknown3.375	3.375	4.2	ng	83668	1	6.875	395957	20.0
2-Pentanone, 4-...	5.087	5.7	ng	113427	1	6.875	395957	20.0
1-Phenoxypropan...	8.469	2.5	ng	63523	2	8.157	517947	20.0
unknown9.822	9.822	2.3	ng	67376	3	9.910	592273	20.0
unknown10.316	10.316	3.3	ng	97608	3	9.910	592273	20.0