

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
 Data File : BF137022.D
 Acq On : 10 Jan 2024 16:20
 Operator : CG\JU
 Sample : P1085-07
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-4

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137022.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.204	9	20	23	rBV	706521	1025063	66.64%	8.692%
2	3.357	212	216	230	rBV	52368	117152	7.62%	0.993%
3	3.651	262	266	275	rVB4	15925	27444	1.78%	0.233%
4	3.928	308	313	318	rBV3	16849	24754	1.61%	0.210%
5	4.016	323	328	330	rBV	18622	26655	1.73%	0.226%
6	4.040	330	332	343	rVB	22838	33822	2.20%	0.287%
7	4.451	398	402	409	rVB	22428	27081	1.76%	0.230%
8	4.604	424	428	435	rBV	127402	135433	8.80%	1.148%
9	4.769	452	456	466	rBV	34997	50619	3.29%	0.429%
10	5.022	494	499	511	rVB	452520	531797	34.57%	4.509%
11	5.434	565	569	581	rBV	1104914	1004287	65.29%	8.516%
12	6.228	699	704	710	rBV2	12718	19828	1.29%	0.168%
13	6.439	736	740	755	rBV	1311063	1285739	83.59%	10.902%
14	6.622	764	771	775	rBV	27503	33187	2.16%	0.281%
15	6.781	795	798	802	rVB	393643	325061	21.13%	2.756%
16	6.904	817	819	826	rVB2	16560	19087	1.24%	0.162%
17	7.345	890	894	897	rBV	879666	847123	55.07%	7.183%
18	7.598	934	937	943	rBV	43604	34876	2.27%	0.296%
19	8.057	1012	1015	1023	rVB	469261	408490	26.56%	3.464%
20	8.339	1059	1063	1065	rBV2	17170	20651	1.34%	0.175%
21	8.375	1065	1069	1072	rBV2	42581	56529	3.68%	0.479%
22	9.139	1194	1199	1202	rBV	1868418	1538142	100.00%	13.043%
23	9.816	1311	1314	1318	rBV	519169	408310	26.55%	3.462%
24	9.916	1326	1331	1338	rBV	324537	441715	28.72%	3.746%
25	10.469	1421	1425	1429	rVB2	23600	28253	1.84%	0.240%
26	10.610	1446	1449	1460	rBV	504912	478834	31.13%	4.060%
27	10.733	1466	1470	1478	rVB	70883	88823	5.77%	0.753%
28	11.198	1547	1549	1555	rVB2	28060	30268	1.97%	0.257%
29	11.310	1565	1568	1571	rBV	444367	378600	24.61%	3.210%
30	11.333	1571	1572	1576	rVB	53997	33146	2.15%	0.281%
31	11.845	1656	1659	1667	rBV2	92345	98667	6.41%	0.837%
32	12.404	1751	1754	1760	rVB5	12556	19439	1.26%	0.165%
33	12.533	1773	1776	1779	rBV	54978	48936	3.18%	0.415%
34	12.633	1790	1793	1799	rBV4	19008	26853	1.75%	0.228%
35	12.763	1809	1815	1820	rVB	48009	54246	3.53%	0.460%
36	12.910	1835	1840	1843	rBV	1200853	1156830	75.21%	9.809%

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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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.863	1996	2002	2012	rBV7	23125	63027	4.10%	0.534%
38	13.968	2016	2020	2023	rBV	357344	340012	22.11%	2.883%
39	15.021	2196	2199	2202	rBV2	21412	33099	2.15%	0.281%
40	15.086	2208	2210	2215	rVB5	18470	20590	1.34%	0.175%
41	15.398	2259	2263	2267	rVB	20048	25826	1.68%	0.219%
42	15.457	2269	2273	2281	rBV	309940	404608	26.30%	3.431%
43	15.927	2348	2353	2357	rBV7	10933	20267	1.32%	0.172%

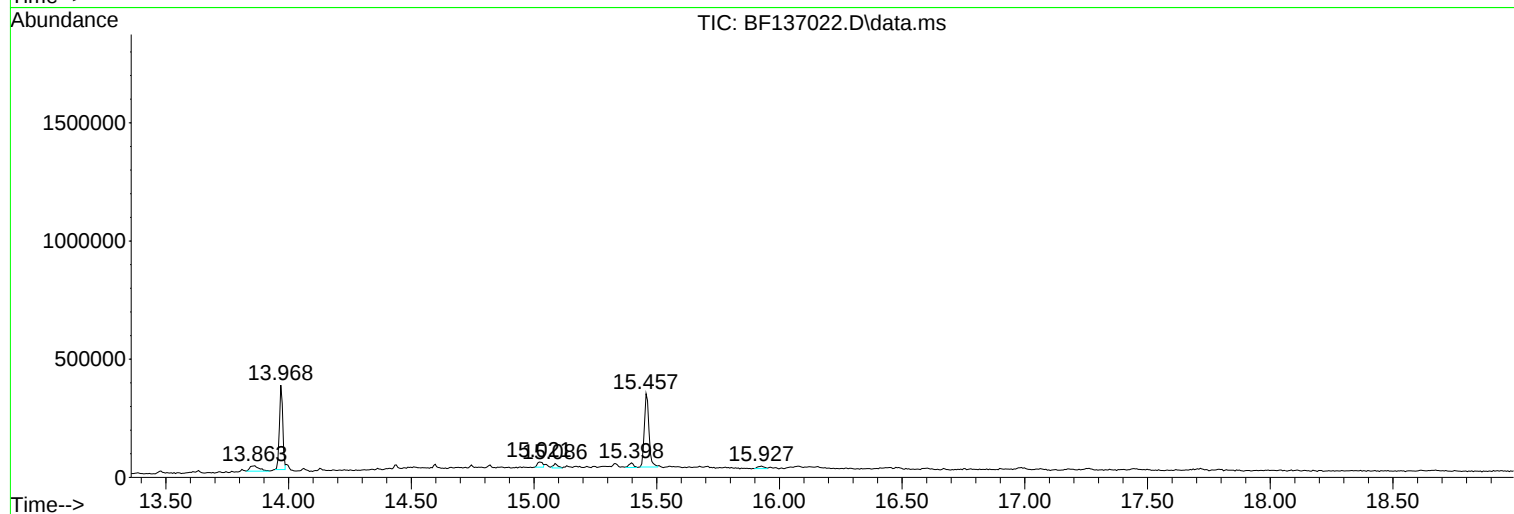
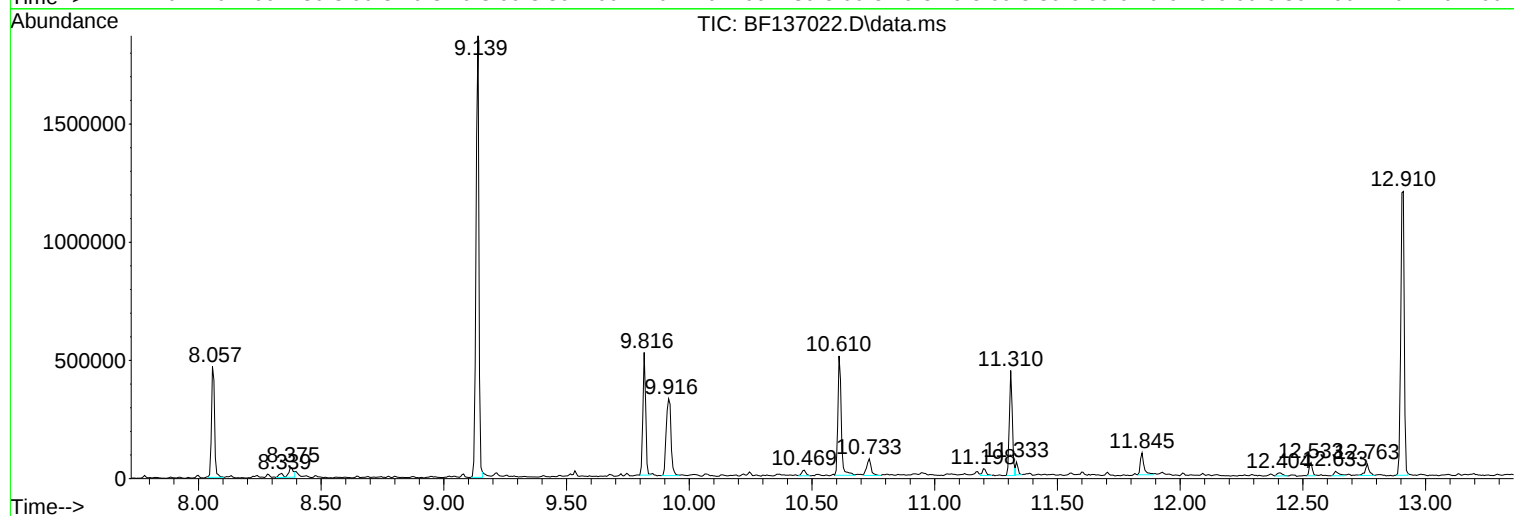
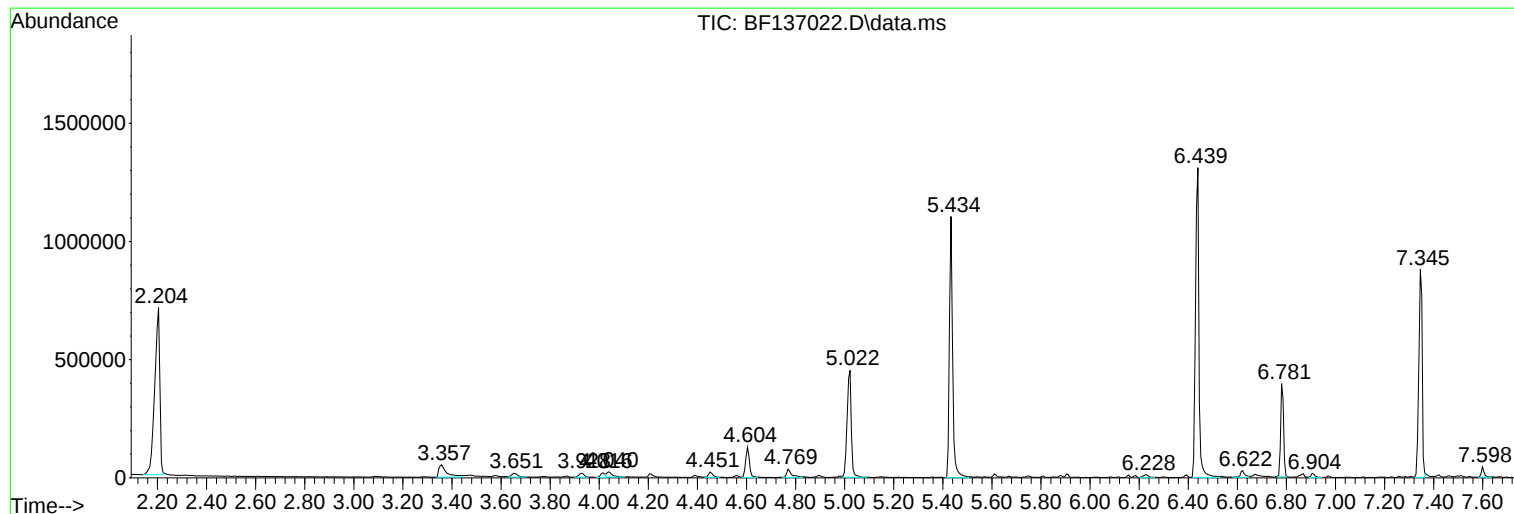
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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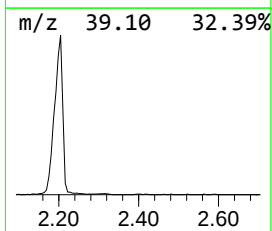
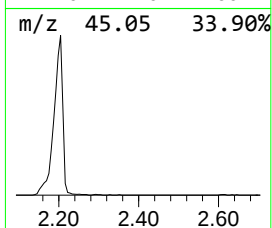
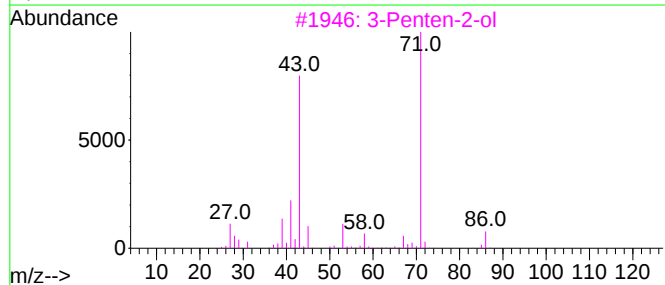
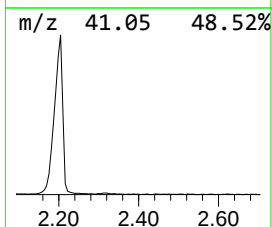
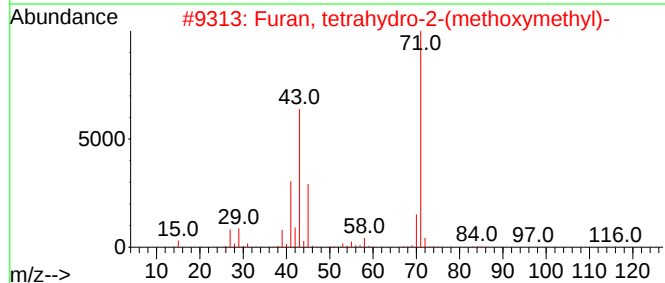
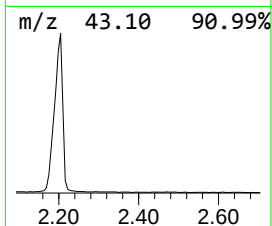
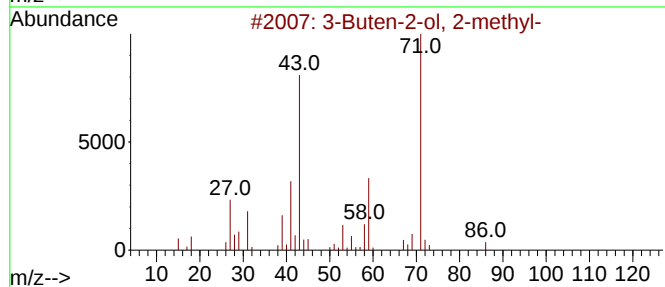
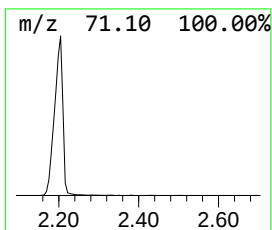
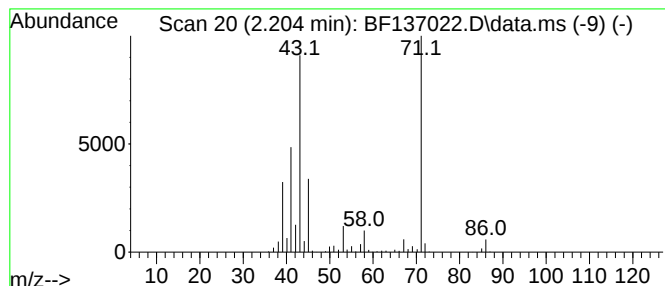
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Buten-2-ol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.204	63.07 ng	1025060	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	72
2			Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	72
3			3-Penten-2-ol	86	C5H10O	001569-50-2	72
4			Butane, 2-bromo-2-methyl-	150	C5H11Br	000507-36-8	53
5			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	45



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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

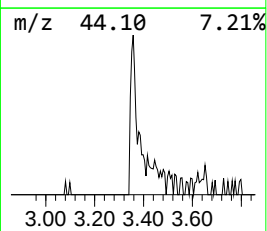
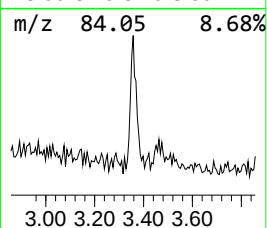
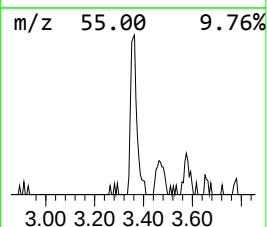
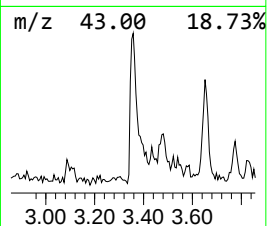
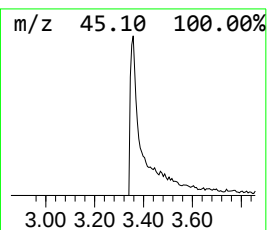
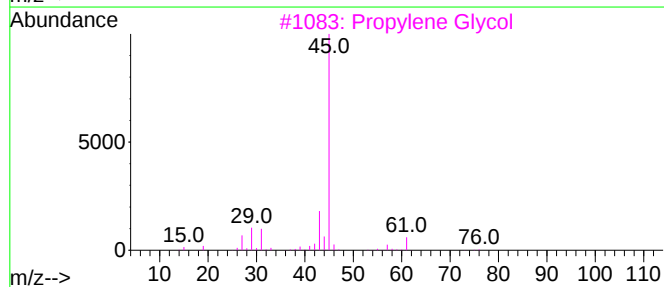
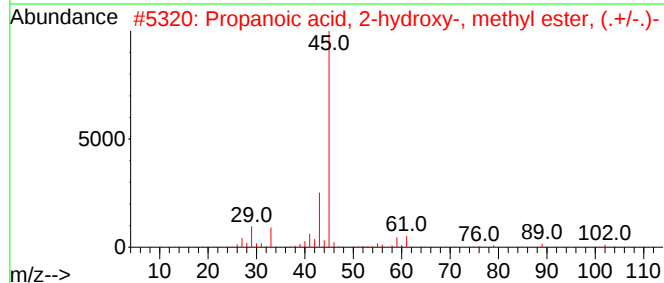
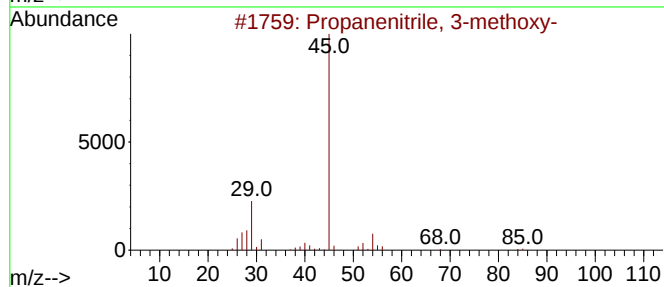
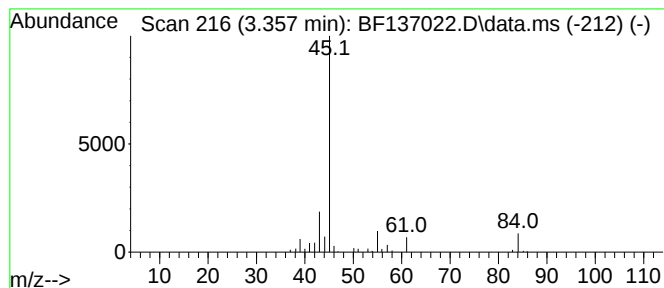
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown3.357 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.357	7.21 ng	117152	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanenitrile, 3-methoxy-	85	C4H7NO	000110-67-8	45
2			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
3			Propylene Glycol	76	C3H8O2	000057-55-6	40
4			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40
5			2-Heptanol	116	C7H16O	000543-49-7	39



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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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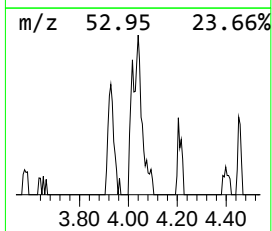
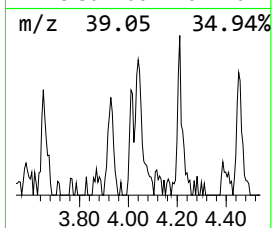
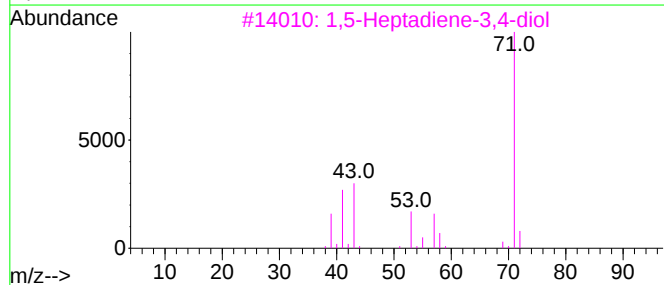
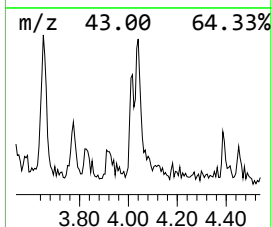
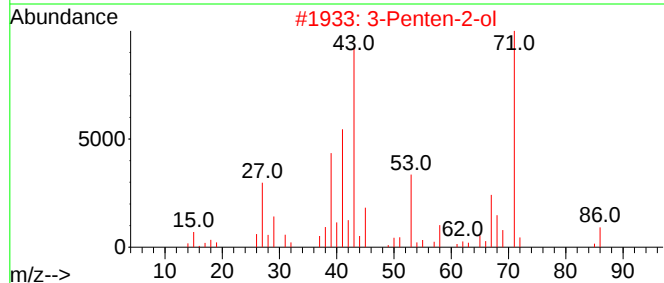
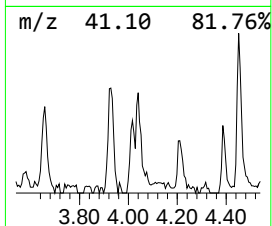
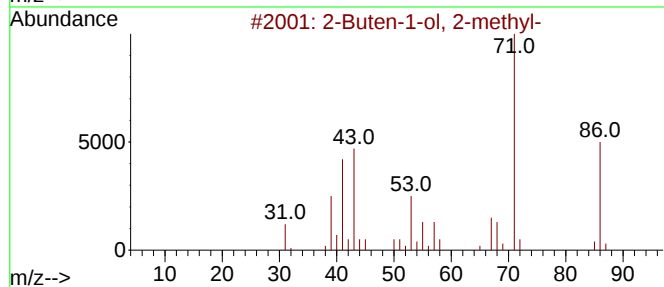
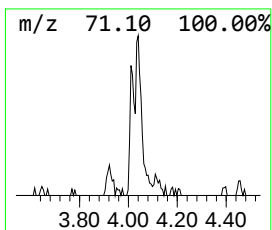
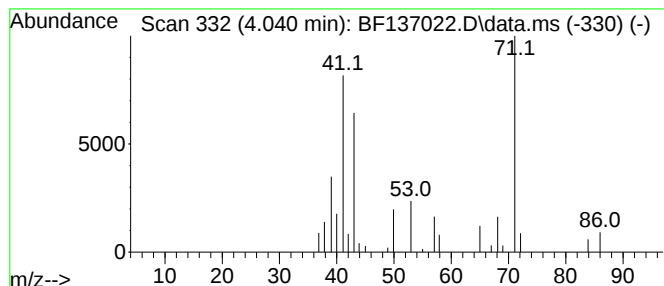
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Buten-1-ol, 2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.040	2.08 ng	33822	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Buten-1-ol, 2-methyl-			86	C5H10O	004675-87-0	64
2	3-Penten-2-ol			86	C5H10O	001569-50-2	58
3	1,5-Heptadiene-3,4-diol			128	C7H12O2	051945-98-3	50
4	Pantolactone			130	C6H10O3	000599-04-2	38
5	Cyclopropanemethanol, .alpha.-bu...			128	C8H16O	004379-16-2	25



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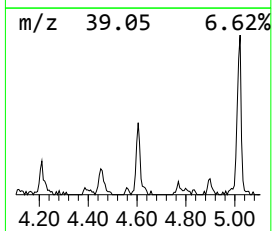
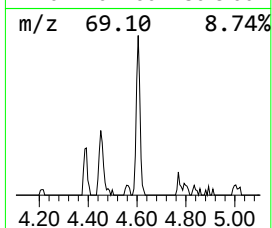
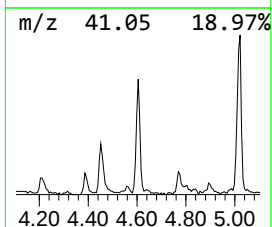
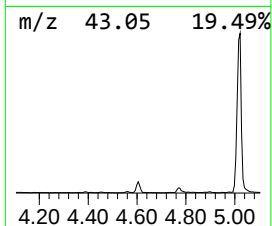
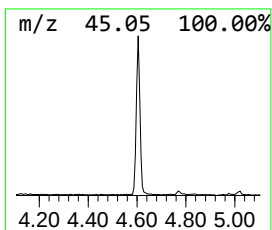
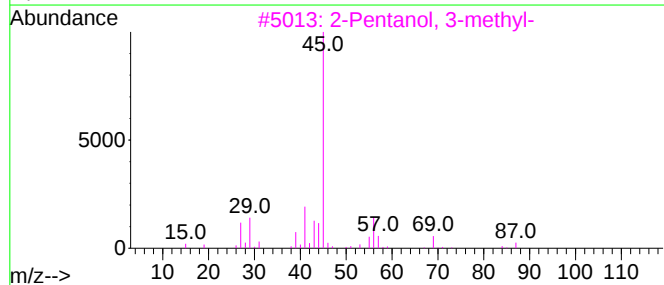
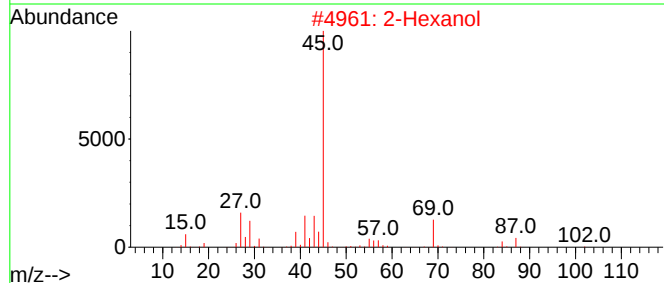
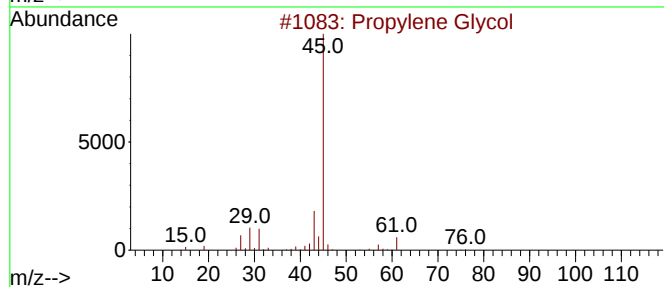
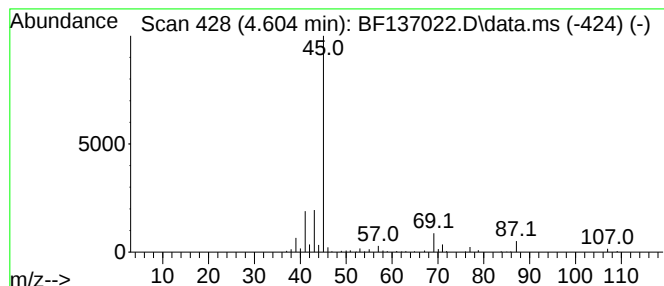
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Propylene Glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.604	8.33 ng	135433	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	64
2			2-Hexanol	102	C6H14O	000626-93-7	40
3			2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	40
4			(R)-(-)-3-Methyl-2-butanol	88	C5H12O	001572-93-6	39
5			4-Penten-2-ol	86	C5H10O	000625-31-0	38



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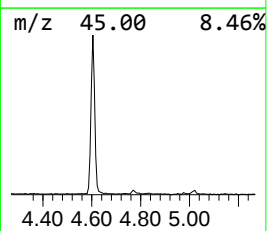
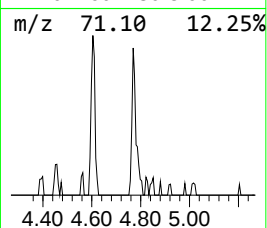
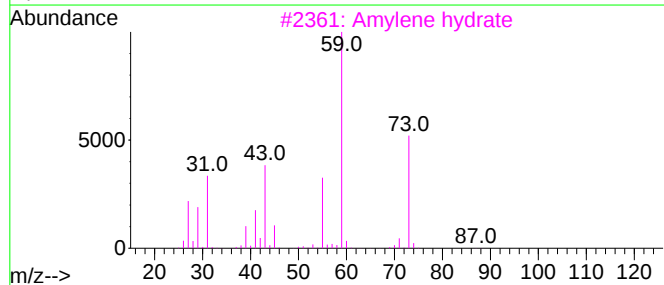
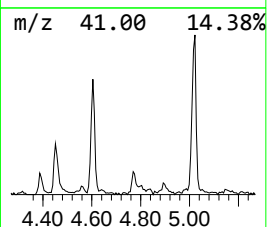
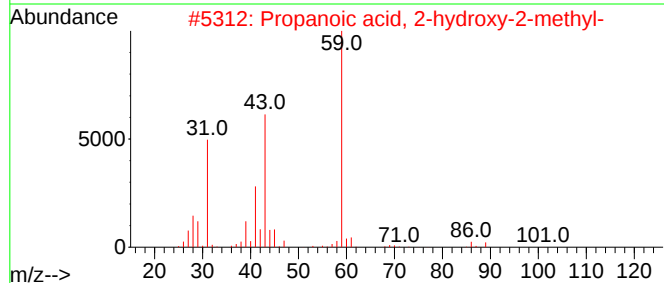
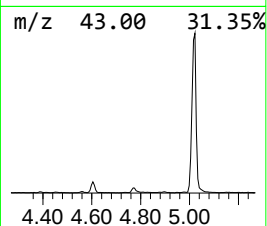
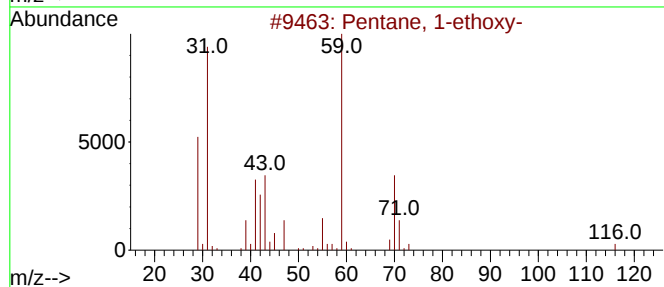
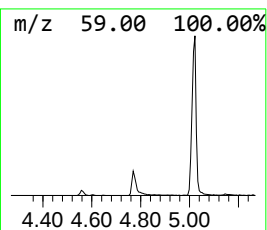
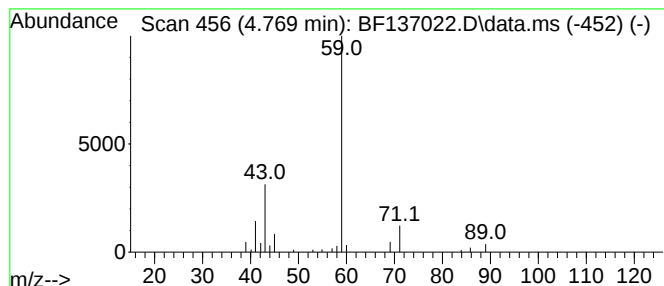
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown4.769 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.769	3.11 ng	50619	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 1-ethoxy-	116	C7H16O	017952-11-3	40
2			Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	39
3			Amylene hydrate	88	C5H12O	000075-85-4	39
4			2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	38
5			Guanidine	59	CH5N3	000113-00-8	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137022.D
Acq On : 10 Jan 2024 16:20
Operator : CG\JU
Sample : P1085-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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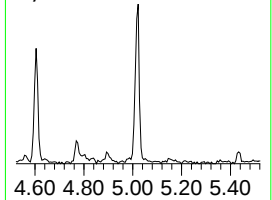
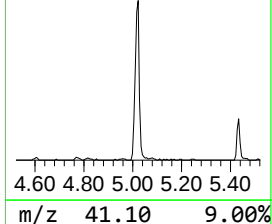
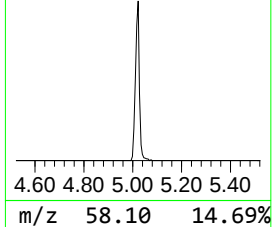
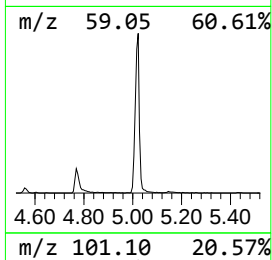
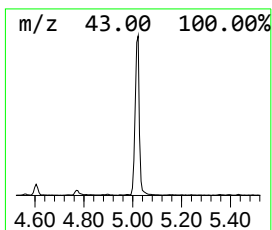
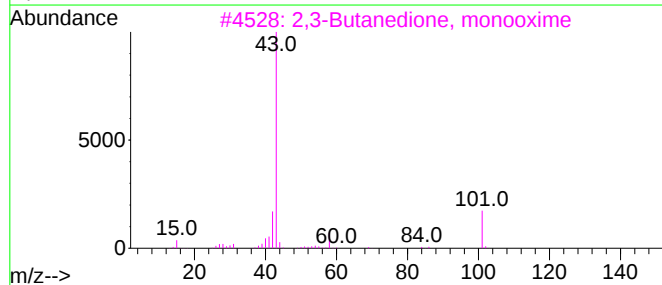
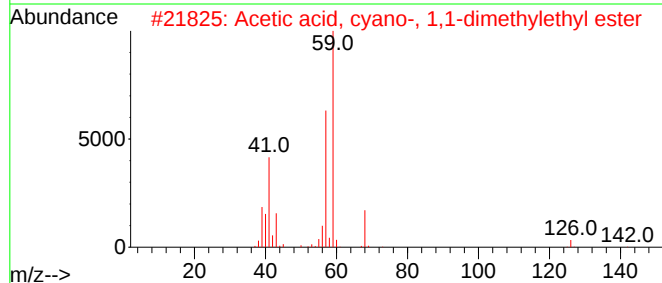
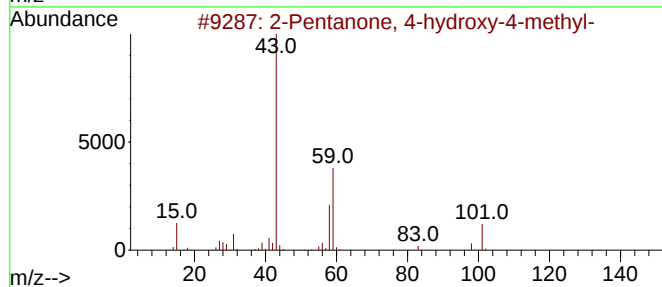
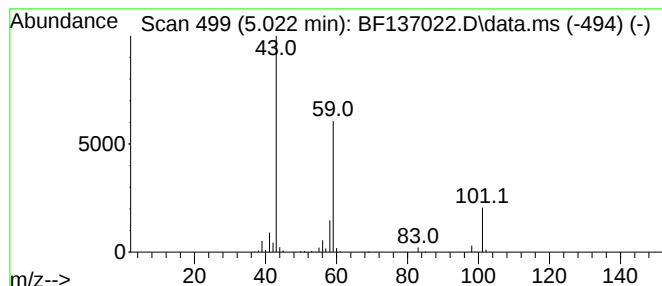
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	32.72 ng	531797	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137022.D
Acq On : 10 Jan 2024 16:20
Operator : CG\JU
Sample : P1085-07
Misc :
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ClientSampleId :
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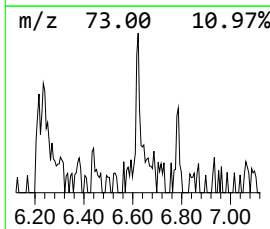
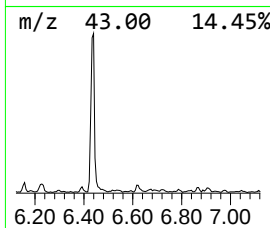
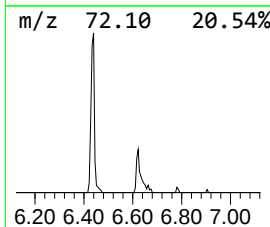
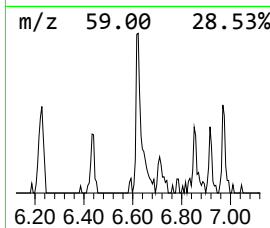
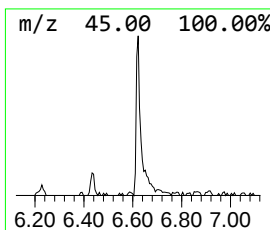
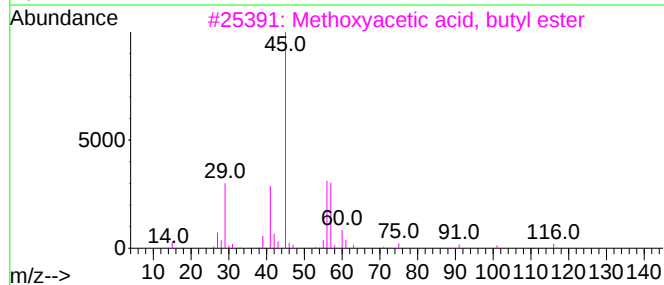
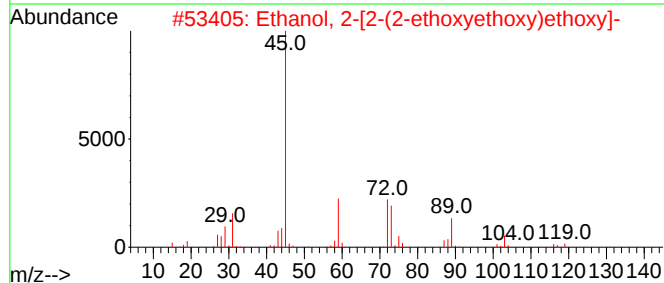
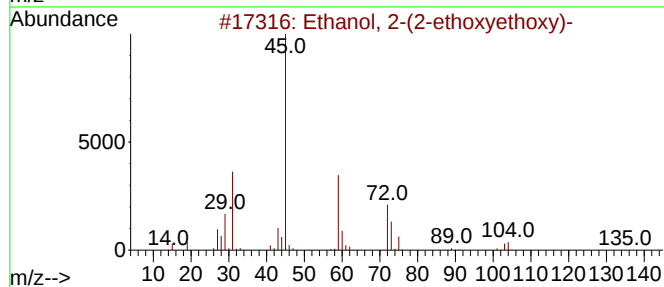
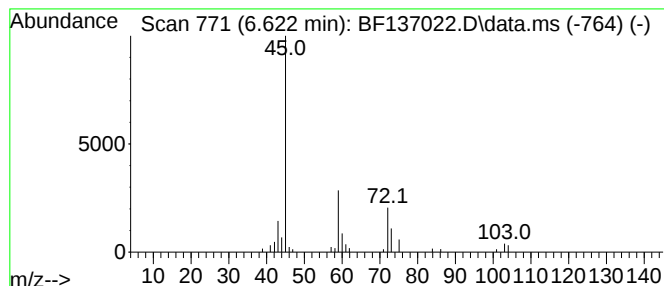
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.622	2.04 ng	33187	1,4-Dichlorobenzene-d4	6.781

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	39
3			Methoxyacetic acid, butyl ester	146	C7H14O3	017640-22-1	38
4			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38
5			Methoxyacetic acid, 2-methylprop...	146	C7H14O3	1000282-40-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137022.D
Acq On : 10 Jan 2024 16:20
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Sample : P1085-07
Misc :
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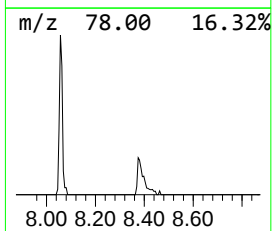
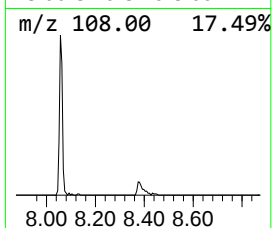
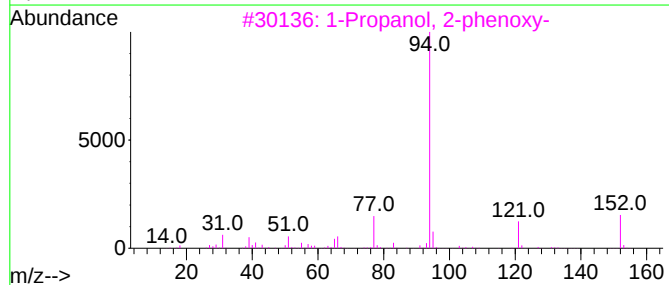
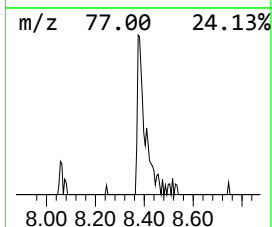
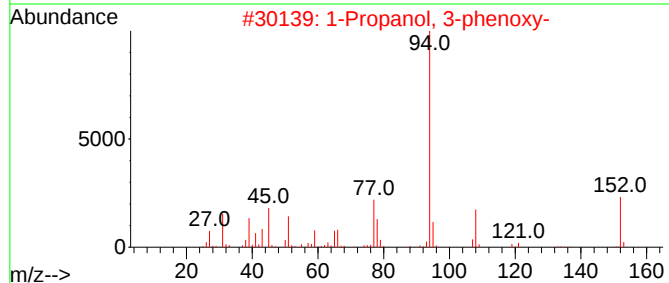
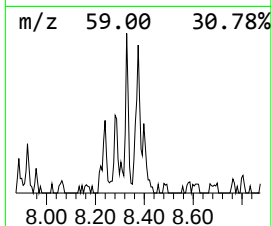
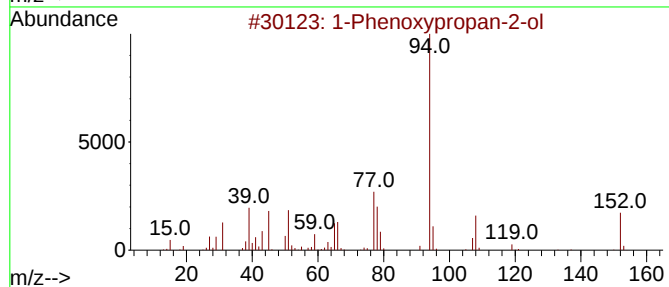
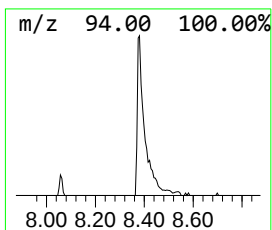
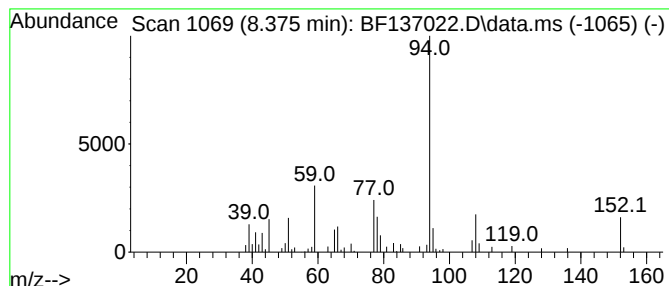
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Phenoxypropan-2-ol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.375	2.77 ng	56529	Naphthalene-d8	8.057

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
2		1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3		1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
4		Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	53
5		Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137022.D
Acq On : 10 Jan 2024 16:20
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Sample : P1085-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

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ClientSampleId :
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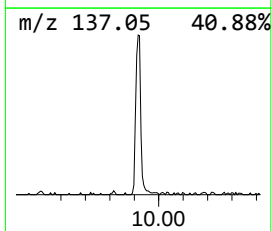
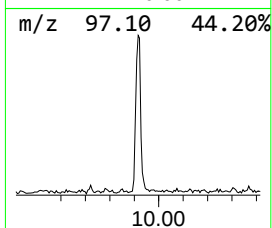
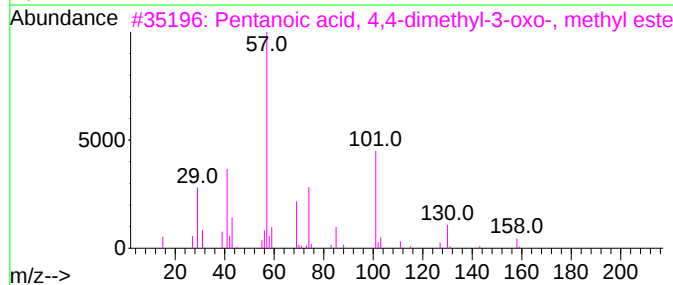
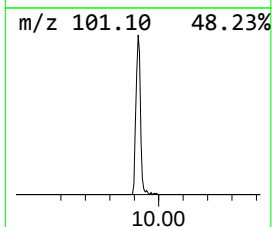
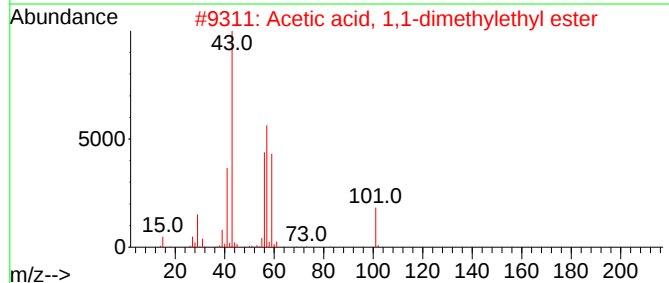
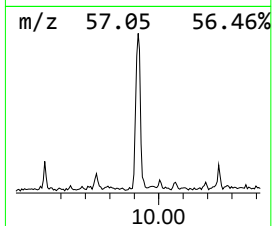
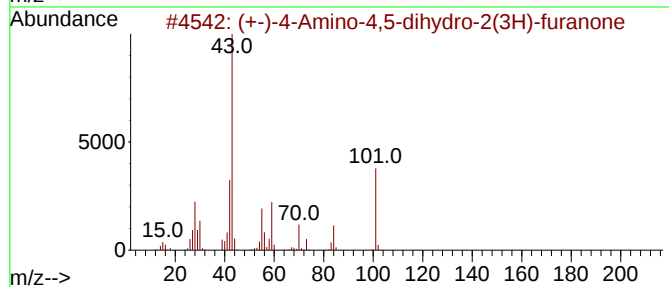
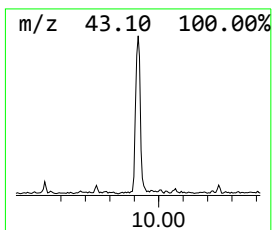
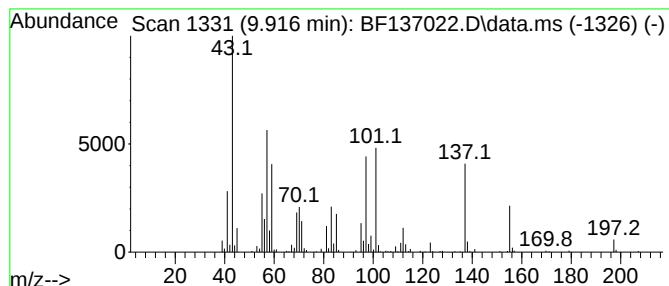
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown9.916 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.916	21.64 ng	441715	Acenaphthene-d10	9.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	16		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	10		
3	Pentanoic acid, 4,4-dimethyl-3-o...	158	C8H14O3	055107-14-7	10		
4	2,4,4-Trimethyl-1-pentanol, chlo...	242	C10H17ClF2O2	1000447-27-2	10		
5	Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137022.D
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Misc :
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Instrument :
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ClientSampleId :
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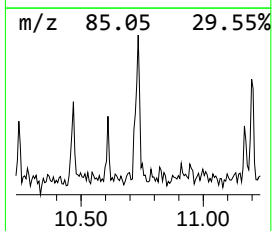
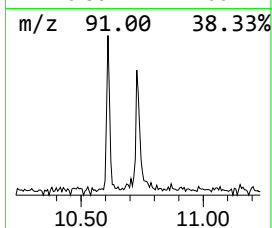
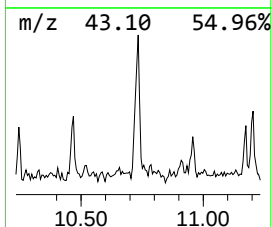
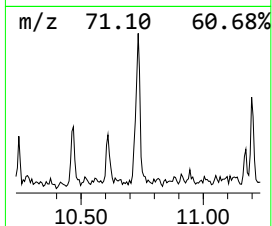
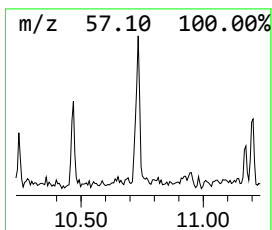
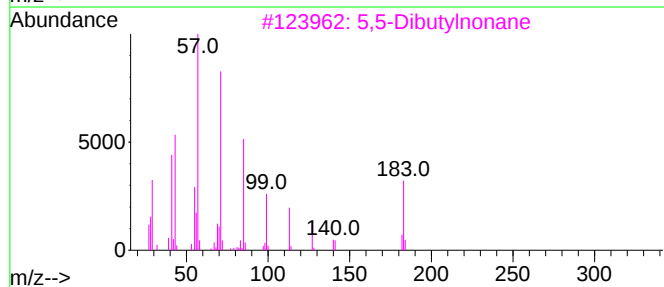
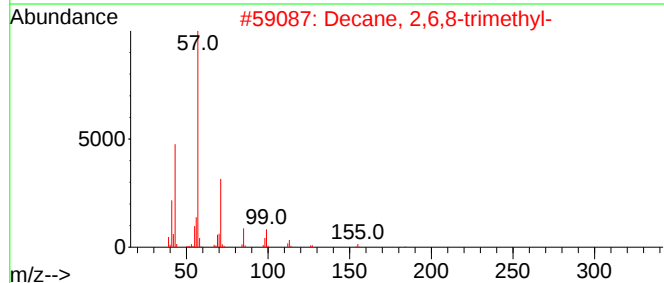
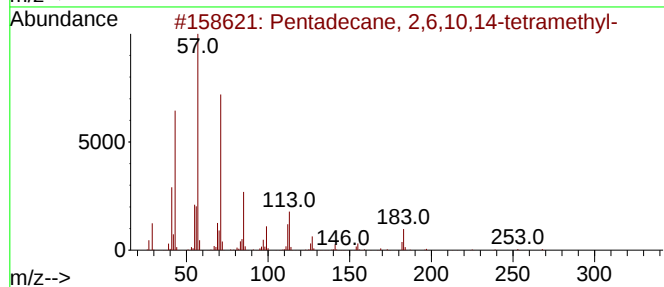
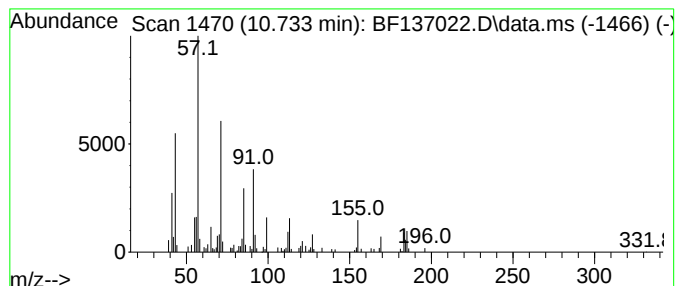
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Pentadecane, 2,6,10,14-tetr... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.733	4.69 ng	88823	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	80
2			Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	62
3			5,5-Dibutylnonane	240	C17H36	006008-17-9	52
4			Decane, 5-ethyl-5-methyl-	184	C13H28	017312-74-2	50
5			Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
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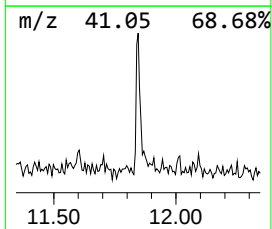
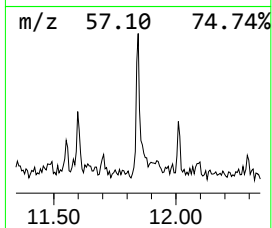
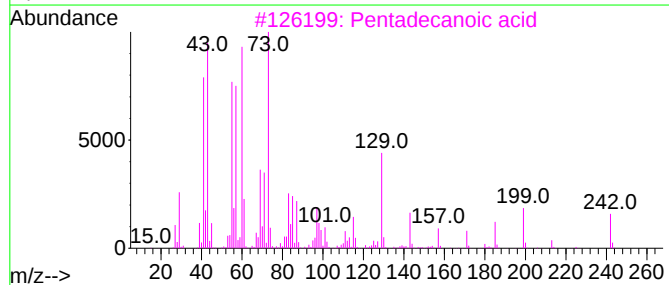
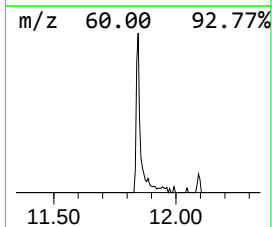
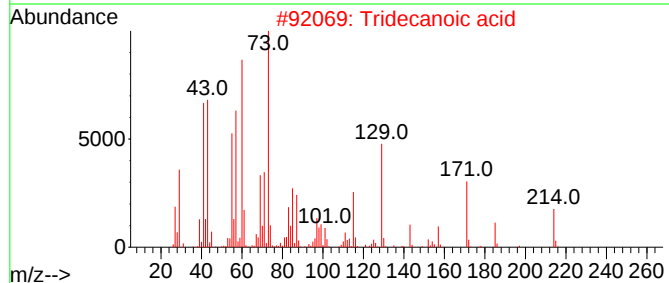
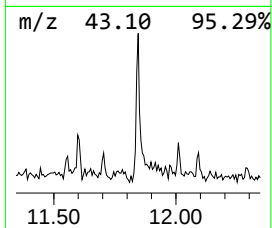
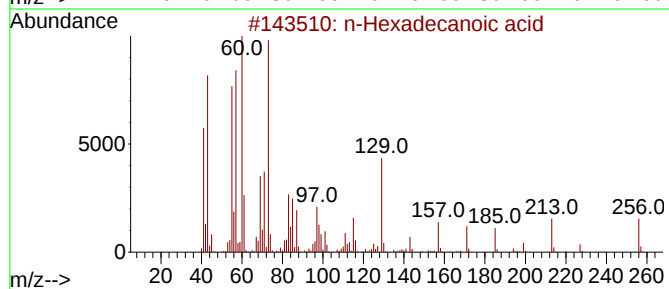
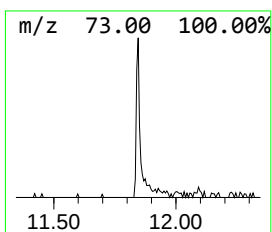
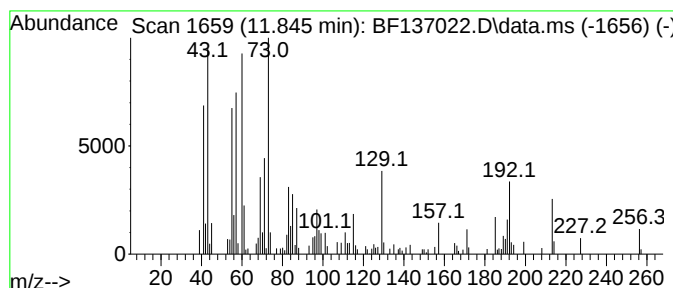
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.845	5.21 ng	98667	Phenanthrene-d10		11.310	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tridecanoic acid		214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	80
5	N-(3,4-Difluorophenyl)-2,2-dimet...		213	C11H13F2NO	1000486-60-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137022.D
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ALS Vial : 13 Sample Multiplier: 1

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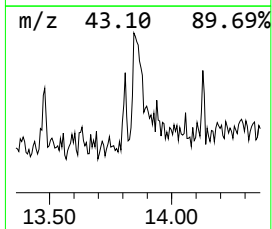
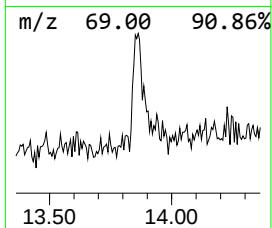
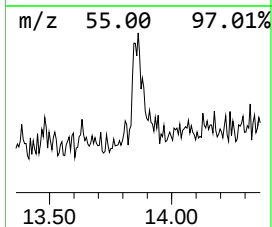
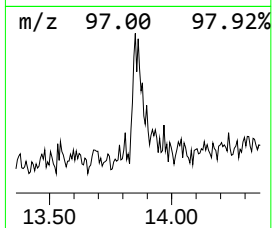
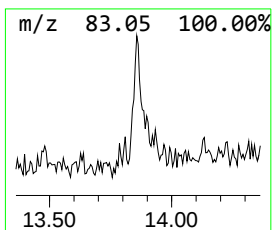
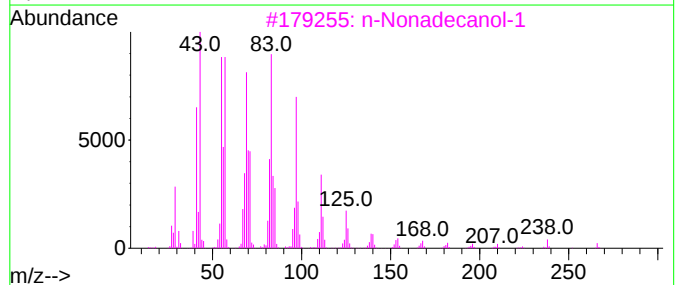
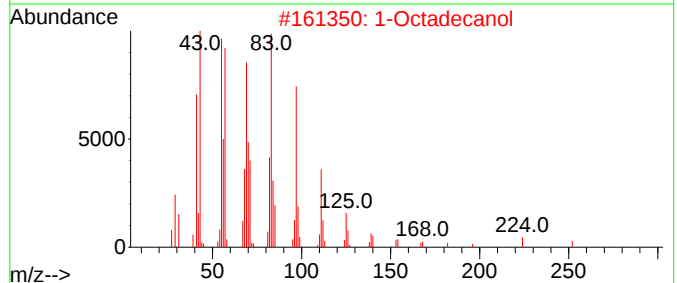
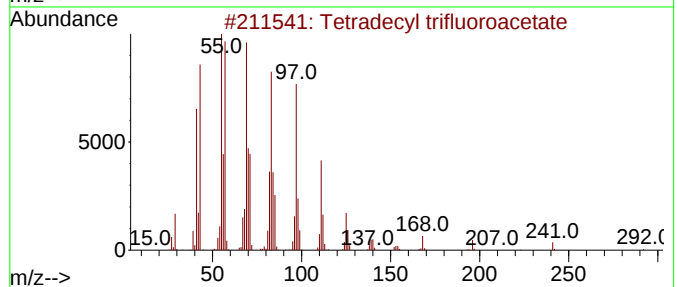
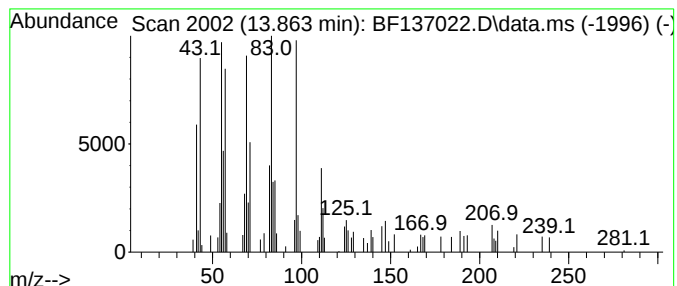
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Tetradecyl trifluoroacetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	3.71 ng	63027	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	91
2			1-Octadecanol	270	C18H38O	000112-92-5	90
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	87
4			1-Nonadecene	266	C19H38	018435-45-5	87
5			1-Heneicosanol	312	C21H44O	015594-90-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137022.D
Acq On : 10 Jan 2024 16:20
Operator : CG\JU
Sample : P1085-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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
3-Buten-2-ol, 2...	2.204	63.1	ng	1025060	1	6.781	325061	20.0
unknown3.357	3.357	7.2	ng	117152	1	6.781	325061	20.0
2-Buten-1-ol, 2...	4.040	2.1	ng	33822	1	6.781	325061	20.0
Propylene Glycol	4.604	8.3	ng	135433	1	6.781	325061	20.0
unknown4.769	4.769	3.1	ng	50619	1	6.781	325061	20.0
2-Pentanone, 4-...	5.022	32.7	ng	531797	1	6.781	325061	20.0
Ethanol, 2-(2-e...	6.622	2.0	ng	33187	1	6.781	325061	20.0
1-Phenoxypropan...	8.375	2.8	ng	56529	2	8.057	408490	20.0
unknown9.916	9.916	21.6	ng	441715	3	9.816	408310	20.0
Pentadecane, 2,...	10.733	4.7	ng	88823	4	11.310	378600	20.0
n-Hexadecanoic ...	11.845	5.2	ng	98667	4	11.310	378600	20.0
Tetradecyl trif...	13.863	3.7	ng	63027	5	13.968	340012	20.0