

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
 Data File : BF137021.D
 Acq On : 10 Jan 2024 15:47
 Operator : CG\JU
 Sample : P1085-05
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-3

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: BF137021.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	6	16	25	rBV	527149	730620	76.88%	8.783%
2	3.357	210	216	228	rBV5	9407	31819	3.35%	0.383%
3	3.646	261	265	271	rVB5	6409	10771	1.13%	0.129%
4	3.922	307	312	316	rVB3	10920	15875	1.67%	0.191%
5	4.004	323	326	328	rBV2	11686	13162	1.39%	0.158%
6	4.034	328	331	335	rVB3	11004	16015	1.69%	0.193%
7	4.204	357	360	366	rBV4	9911	14007	1.47%	0.168%
8	4.445	396	401	407	rVB2	16949	21194	2.23%	0.255%
9	4.598	423	427	436	rVB	85466	93969	9.89%	1.130%
10	4.763	452	455	459	rBV	17080	20501	2.16%	0.246%
11	5.016	493	498	510	rVB	59611	80400	8.46%	0.967%
12	5.428	565	568	587	rBV	885705	871240	91.68%	10.474%
13	6.222	699	703	706	rBV3	10472	12942	1.36%	0.156%
14	6.434	736	739	755	rBV	932913	836736	88.05%	10.059%
15	6.616	766	770	776	rBV3	10232	18435	1.94%	0.222%
16	6.781	795	798	802	rBV	350203	284549	29.94%	3.421%
17	6.904	815	819	826	rVB3	12746	16236	1.71%	0.195%
18	7.345	890	894	897	rBV	643413	529486	55.72%	6.365%
19	7.598	935	937	943	rVB	21459	18375	1.93%	0.221%
20	8.057	1012	1015	1018	rBV	410359	328474	34.56%	3.949%
21	8.239	1040	1046	1051	rBV6	8177	12045	1.27%	0.145%
22	8.339	1059	1063	1066	rBV3	12095	18641	1.96%	0.224%
23	8.381	1066	1070	1071	rBV3	17925	21106	2.22%	0.254%
24	8.475	1084	1086	1088	rBV	13170	11393	1.20%	0.137%
25	8.775	1134	1137	1139	rBV	18784	16008	1.68%	0.192%
26	8.875	1150	1154	1161	rBV	16334	17895	1.88%	0.215%
27	9.075	1186	1188	1194	rVB2	13956	13615	1.43%	0.164%
28	9.133	1194	1198	1207	rBV	1099889	950316	100.00%	11.424%
29	9.210	1207	1211	1214	rVV2	18439	21192	2.23%	0.255%
30	9.404	1241	1244	1248	rBV5	7938	12689	1.34%	0.153%
31	9.475	1253	1256	1258	rBV	13599	15023	1.58%	0.181%
32	9.533	1264	1266	1268	rVB2	18194	12599	1.33%	0.151%
33	9.680	1288	1291	1292	rBV2	14843	14631	1.54%	0.176%
34	9.745	1300	1302	1305	rBV2	15383	13177	1.39%	0.158%
35	9.816	1311	1314	1318	rVB	430841	337807	35.55%	4.061%
36	9.851	1318	1320	1323	rVB4	10805	11479	1.21%	0.138%

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	9.922	1327	1332	1336	rVB3	17260	23602	2.48%	0.284%
38	10.022	1347	1349	1354	rVB3	10835	10531	1.11%	0.127%
39	10.222	1380	1383	1385	rBV4	13243	13502	1.42%	0.162%
40	10.245	1385	1387	1389	rVV2	17086	11659	1.23%	0.140%
41	10.357	1404	1406	1409	rBV4	10289	10721	1.13%	0.129%
42	10.469	1421	1425	1428	rBV	15135	15417	1.62%	0.185%
43	10.527	1431	1435	1437	rBV4	11012	14036	1.48%	0.169%
44	10.610	1446	1449	1459	rBV	492759	481787	50.70%	5.792%
45	10.733	1466	1470	1475	rVB	68782	88971	9.36%	1.070%
46	11.169	1542	1544	1547	rBV3	11398	13966	1.47%	0.168%
47	11.204	1548	1550	1556	rVB4	20603	22835	2.40%	0.275%
48	11.310	1565	1568	1571	rBV	387258	320190	33.69%	3.849%
49	11.333	1571	1572	1576	rVB	44409	29731	3.13%	0.357%
50	11.845	1656	1659	1663	rBV2	91404	87433	9.20%	1.051%
51	12.010	1685	1687	1692	rBV2	16254	16969	1.79%	0.204%
52	12.404	1752	1754	1756	rVB2	14760	11638	1.22%	0.140%
53	12.533	1773	1776	1780	rBV	61702	53401	5.62%	0.642%
54	12.633	1791	1793	1799	rBV6	18393	18266	1.92%	0.220%
55	12.763	1813	1815	1821	rVB	52209	53745	5.66%	0.646%
56	12.904	1836	1839	1843	rBV	841947	752236	79.16%	9.043%
57	13.974	2017	2021	2023	rBV	318704	327747	34.49%	3.940%
58	15.027	2197	2200	2203	rBV	28629	37389	3.93%	0.449%
59	15.398	2260	2263	2268	rVB	36066	42827	4.51%	0.515%
60	15.462	2269	2274	2281	rBV	300848	382075	40.21%	4.593%
61	16.598	2463	2467	2468	rBV3	11325	13219	1.39%	0.159%

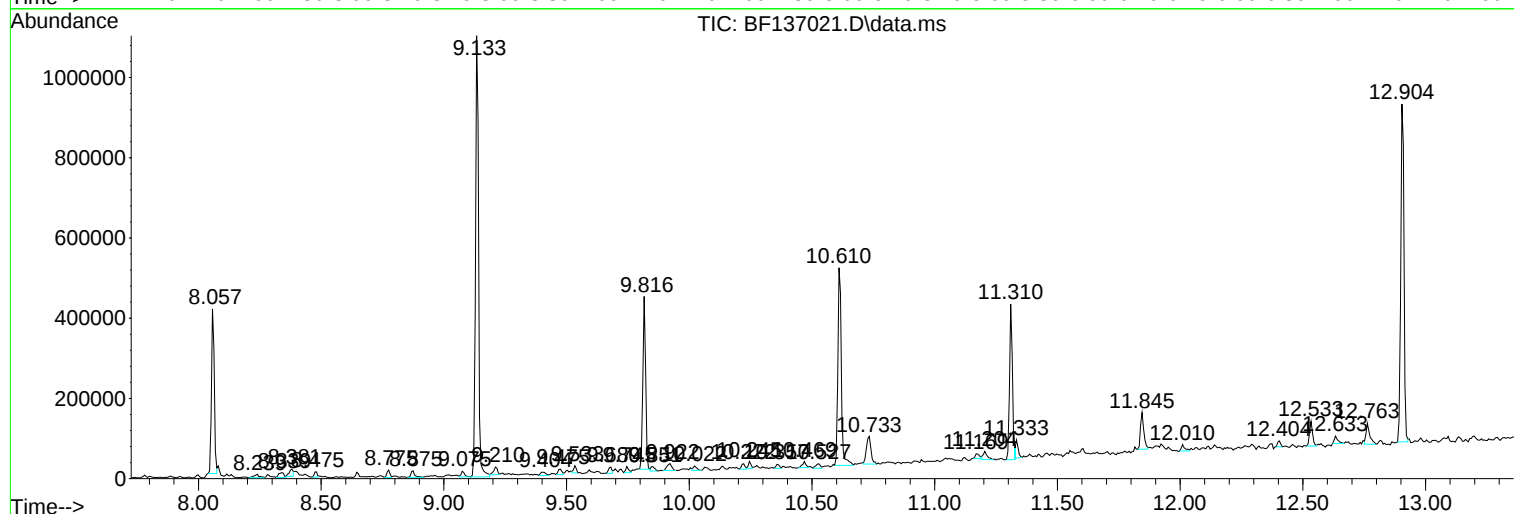
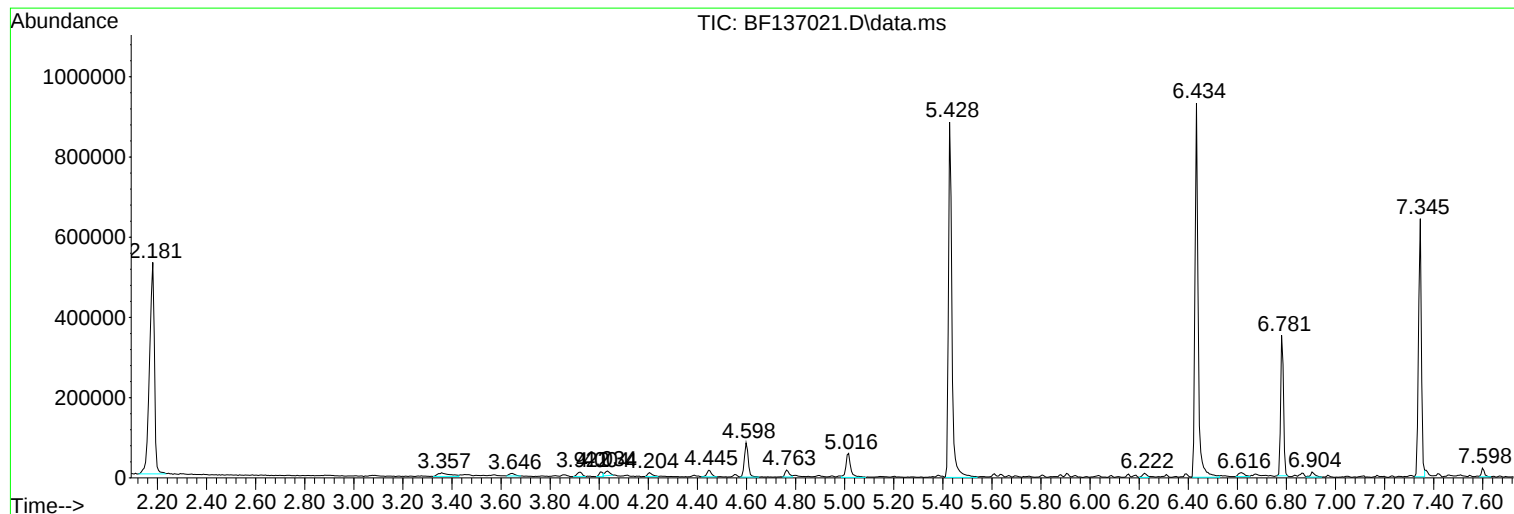
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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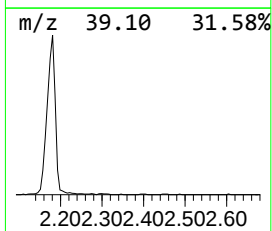
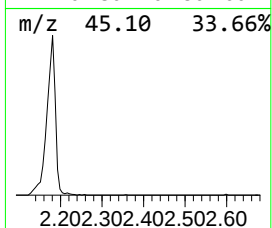
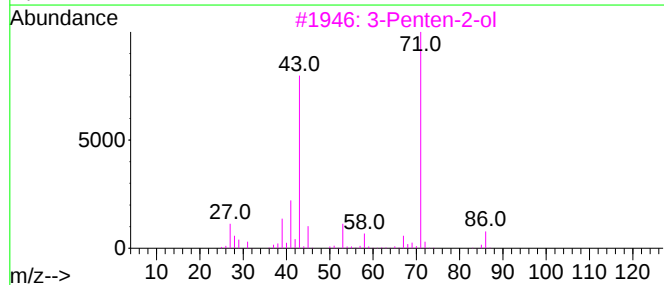
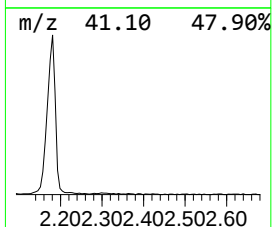
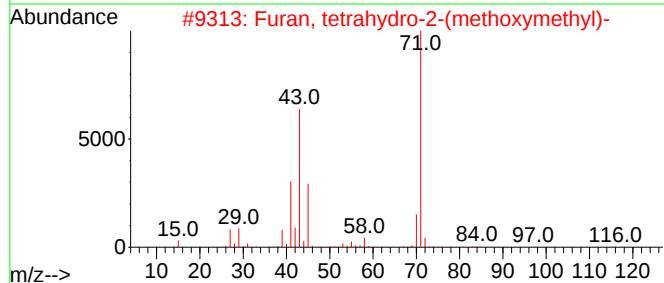
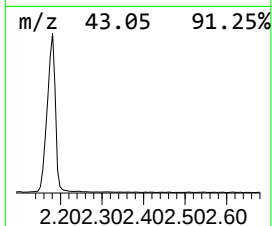
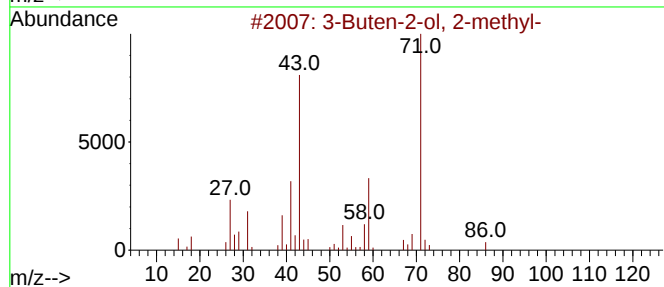
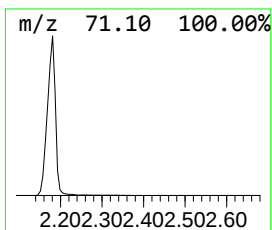
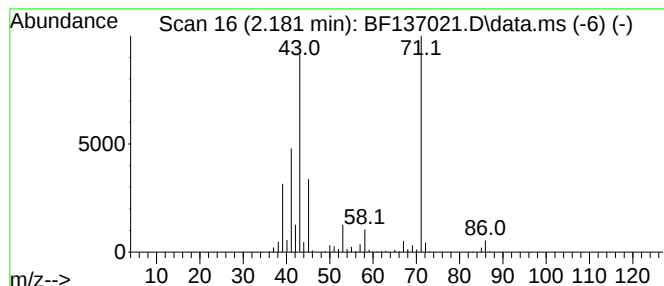
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.181	51.35 ng	730620	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	64
4			Butane, 2-bromo-2-methyl-	150	C5H11Br	000507-36-8	53
5			Furan-2-carbonyl chloride, tetra...	134	C5H7ClO2	052449-98-6	50



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TP-3

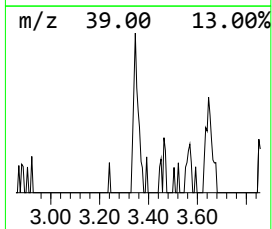
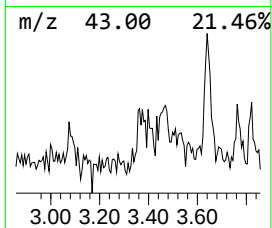
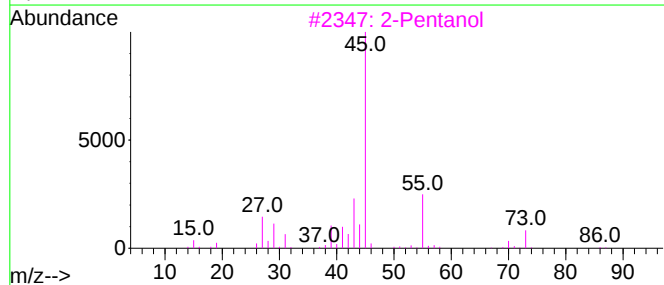
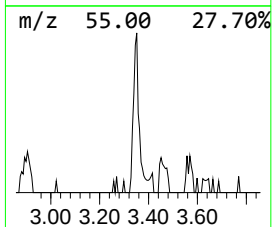
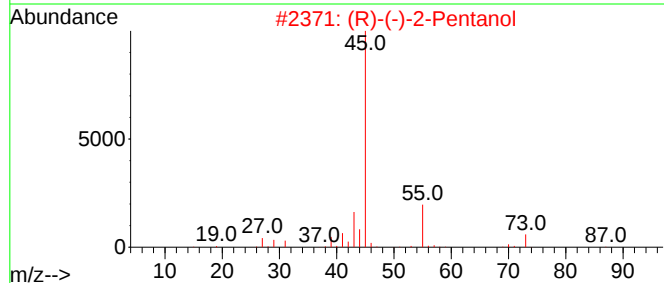
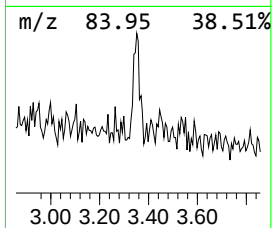
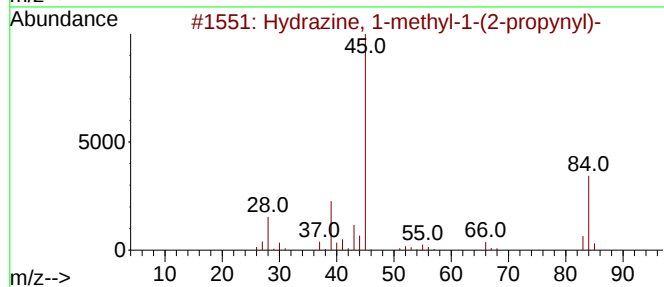
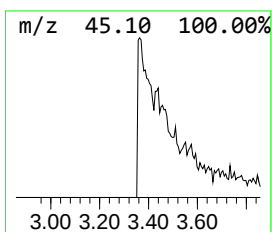
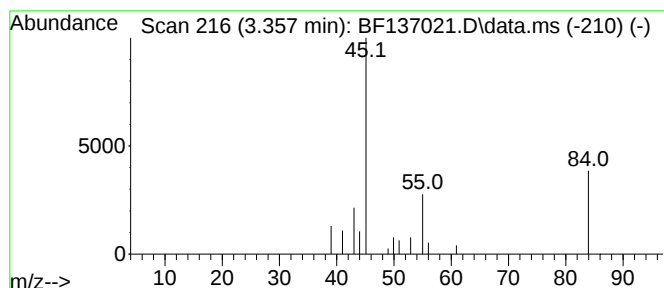
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown3.357 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.357	2.24 ng	31819	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydrazine, 1-methyl-1-(2-propynyl)-	84	C4H8N2	007422-82-4	7
2			(R)-(-)-2-Pentanol	88	C5H12O	031087-44-2	4
3			2-Pentanol	88	C5H12O	006032-29-7	4
4			Methane, nitroso-	45	CH3NO	000865-40-7	3
5			Ethylamine	45	C2H7N	000075-04-7	3



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Misc :
ALS Vial : 12 Sample Multiplier: 1

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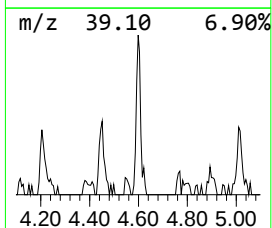
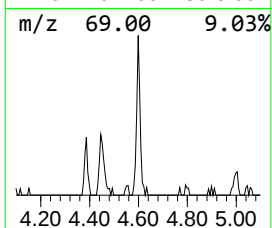
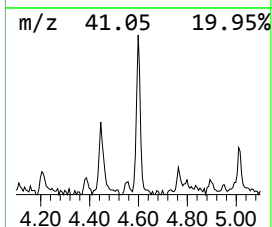
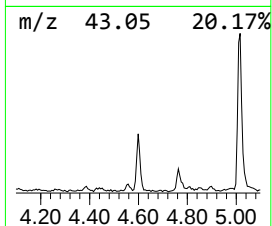
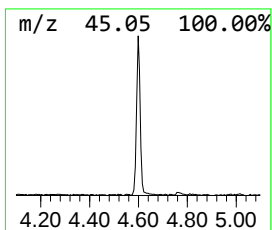
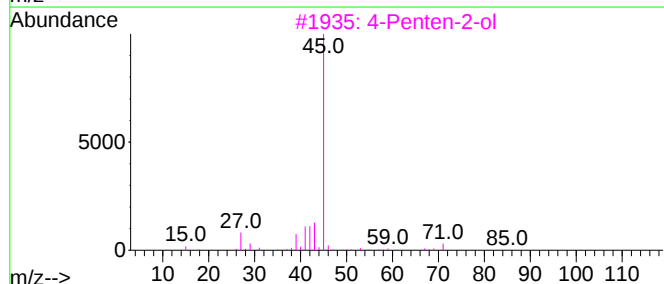
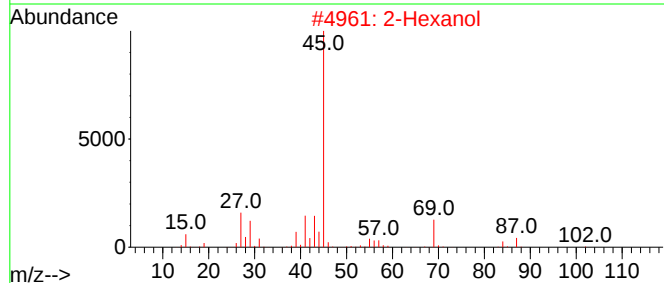
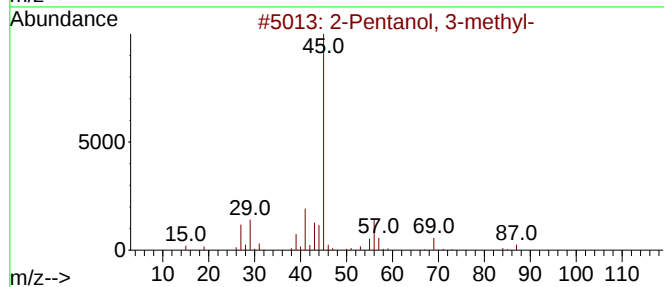
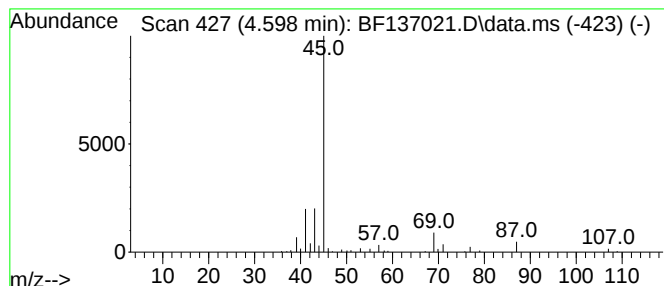
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown4.598 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.598	6.60 ng	93969	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 3-methyl-			102	C6H14O	000565-60-6	40
2	2-Hexanol			102	C6H14O	000626-93-7	40
3	4-Penten-2-ol			86	C5H10O	000625-31-0	38
4	Propylene Glycol			76	C3H8O2	000057-55-6	38
5	2-Pentanol, 4-methyl-			102	C6H14O	000108-11-2	38



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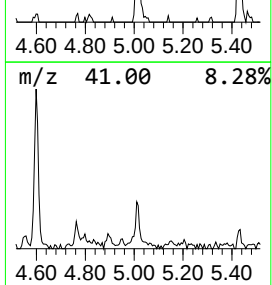
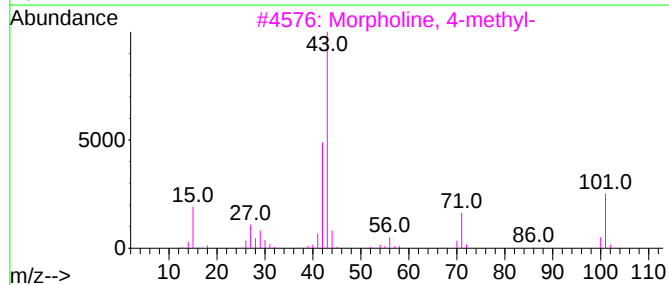
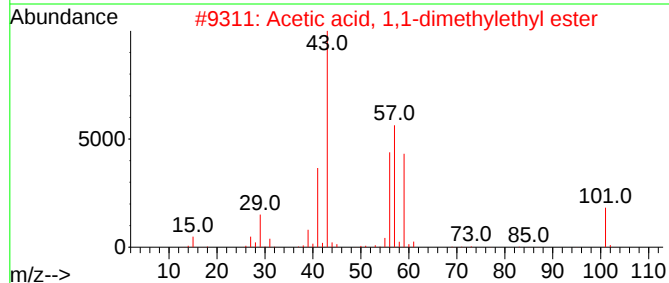
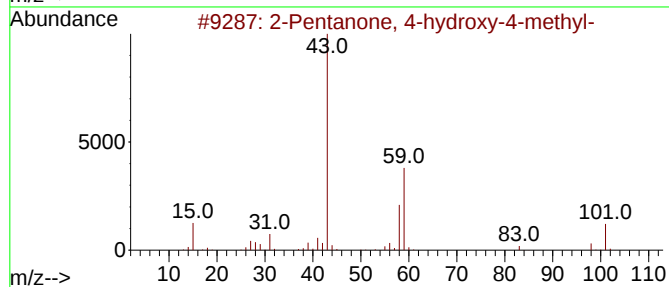
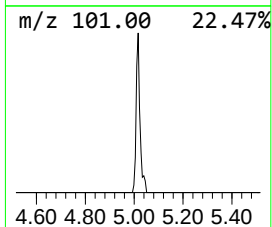
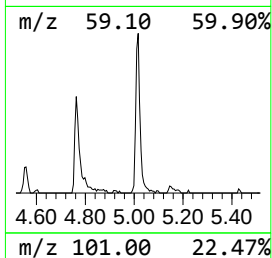
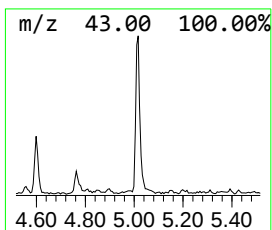
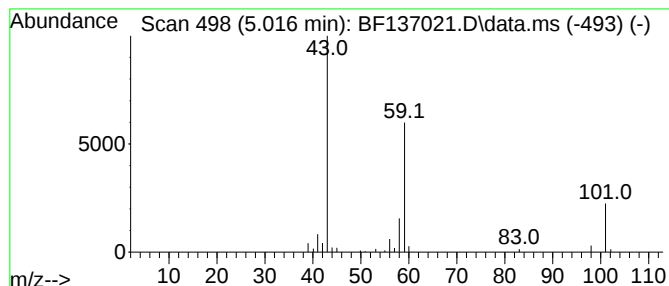
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	5.65 ng	80400	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	56		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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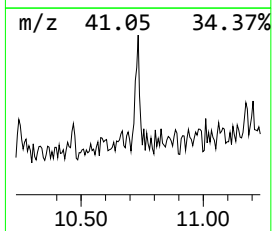
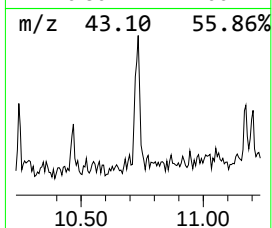
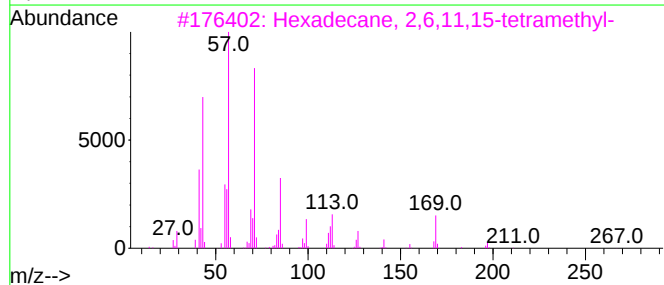
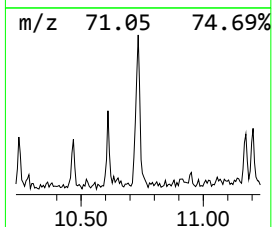
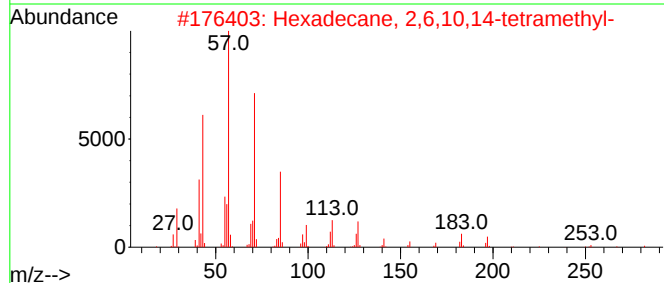
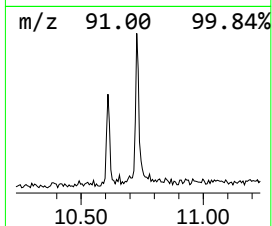
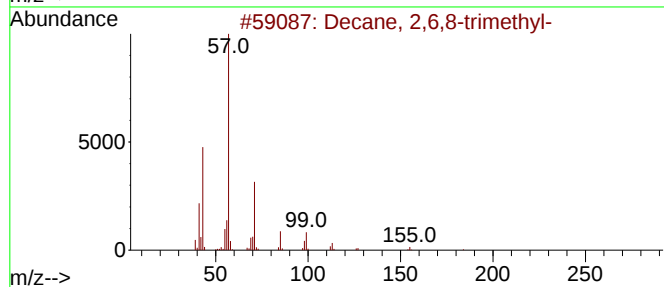
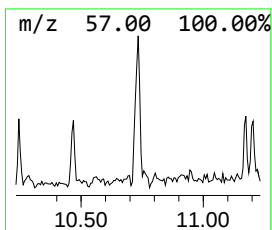
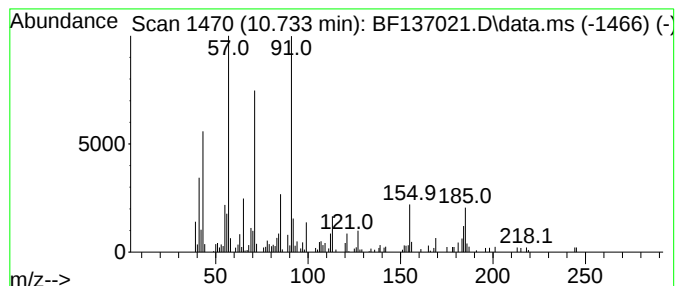
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Decane, 2,6,8-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.733	5.56 ng	88971	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	70
2			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	52
3			Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	52
4			Tridecane	184	C13H28	000629-50-5	50
5			Undeca-4,8-dione	184	C11H20O2	013505-35-6	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137021.D
Acq On : 10 Jan 2024 15:47
Operator : CG\JU
Sample : P1085-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

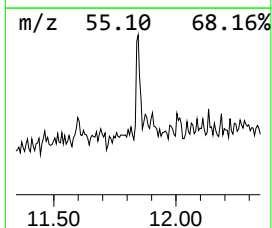
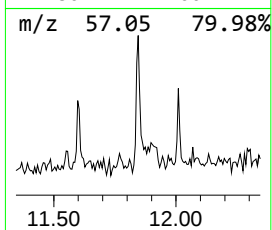
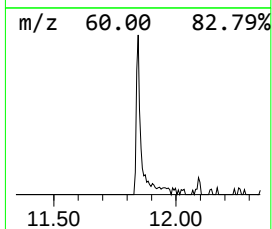
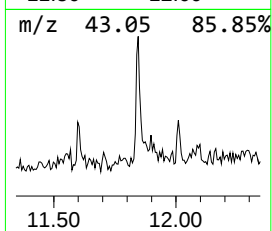
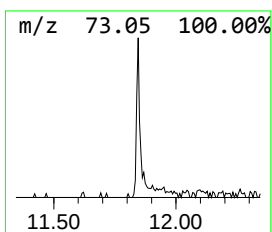
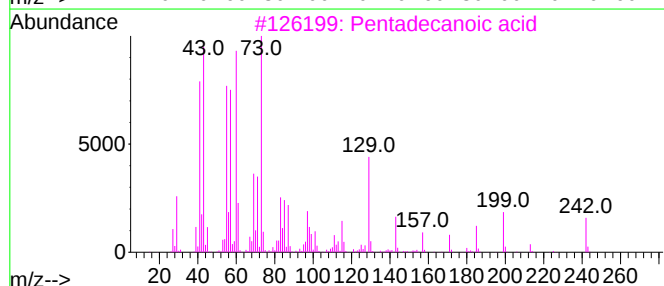
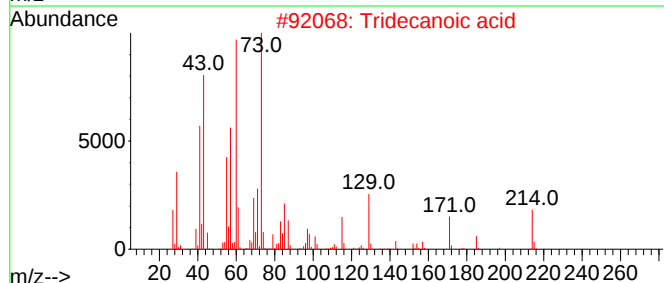
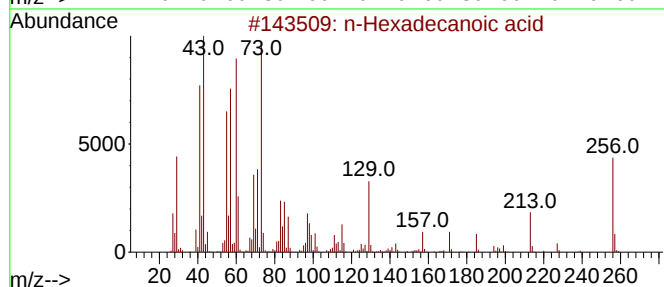
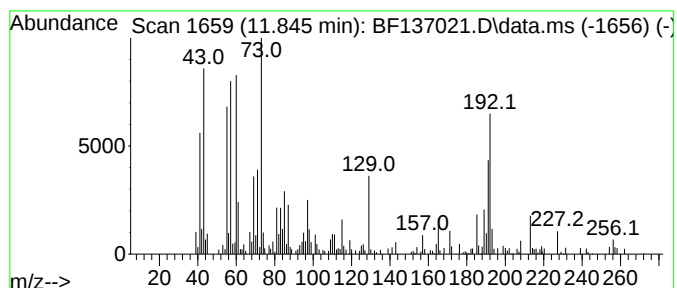
Instrument :
BNA_F
ClientSampleId :
TP-3

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.845	5.46 ng	87433	Phenanthrene-d10		11.310	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	92
2	Tridecanoic acid		214	C13H26O2	000638-53-9	83
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	64
4	Undecanoic acid		186	C11H22O2	000112-37-8	49
5	Nonanoic acid		158	C9H18O2	000112-05-0	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137021.D
Acq On : 10 Jan 2024 15:47
Operator : CG\JU
Sample : P1085-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

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...	2.181	51.4	ng	730620	1	6.781	284549	20.0
unknown3.357	3.357	2.2	ng	31819	1	6.781	284549	20.0
unknown4.598	4.598	6.6	ng	93969	1	6.781	284549	20.0
2-Pentanone, 4-...	5.016	5.7	ng	80400	1	6.781	284549	20.0
Decane, 2,6,8-t...	10.733	5.6	ng	88971	4	11.310	320190	20.0
n-Hexadecanoic ...	11.845	5.5	ng	87433	4	11.310	320190	20.0