

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032422\
 Data File : BF127502.D
 Acq On : 24 Mar 2022 14:57
 Operator : CG\JU
 Sample : N2062-04
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-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-BF032122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127502.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.340	174	179	188	rBV	20713	42436	1.25%	0.240%
2	5.081	472	475	486	rBV	35241	50721	1.50%	0.287%
3	5.475	539	542	563	rBV	1492700	1567378	46.22%	8.867%
4	6.481	710	713	726	rBV	995045	1087723	32.07%	6.154%
5	6.846	772	775	782	rVB	656255	530373	15.64%	3.000%
6	6.904	782	785	791	rBV	38503	47061	1.39%	0.266%
7	7.287	839	850	860	rBV9	15464	55467	1.64%	0.314%
8	7.416	867	872	875	rBV	2127872	2054868	60.59%	11.625%
9	7.528	888	891	897	rBV	66644	75434	2.22%	0.427%
10	8.034	974	977	986	rBV	136433	196909	5.81%	1.114%
11	8.128	990	993	999	rVV	824242	680204	20.06%	3.848%
12	8.498	1052	1056	1061	rBV3	27346	48684	1.44%	0.275%
13	8.934	1127	1130	1137	rBV2	18566	34802	1.03%	0.197%
14	9.134	1161	1164	1171	rBV5	33600	52107	1.54%	0.295%
15	9.204	1171	1176	1179	rBV	3627827	3391335	100.00%	19.186%
16	9.692	1256	1259	1267	rVB3	27215	42909	1.27%	0.243%
17	9.798	1274	1277	1281	rBV2	31907	38788	1.14%	0.219%
18	9.881	1288	1291	1295	rBV	860468	781287	23.04%	4.420%
19	10.275	1354	1358	1360	rBV2	43947	44397	1.31%	0.251%
20	10.681	1423	1427	1435	rBV	2215854	2066842	60.94%	11.693%
21	11.316	1532	1535	1538	rVB	76568	56482	1.67%	0.320%
22	11.375	1542	1545	1549	rBV	897214	757888	22.35%	4.288%
23	11.528	1569	1571	1576	rBV2	48960	53887	1.59%	0.305%
24	11.751	1606	1609	1612	rVB	81527	59962	1.77%	0.339%
25	11.928	1636	1639	1645	rVB	54289	49651	1.46%	0.281%
26	12.963	1810	1815	1818	rBV	2831941	2528596	74.56%	14.305%
27	13.804	1954	1958	1961	rBV	35839	43444	1.28%	0.246%
28	13.845	1961	1965	1968	rVV	63755	87175	2.57%	0.493%
29	13.880	1968	1971	1976	rVB	86305	101980	3.01%	0.577%
30	14.022	1992	1995	2004	rBV	527309	501778	14.80%	2.839%
31	15.504	2243	2247	2260	rVB	407720	545726	16.09%	3.087%

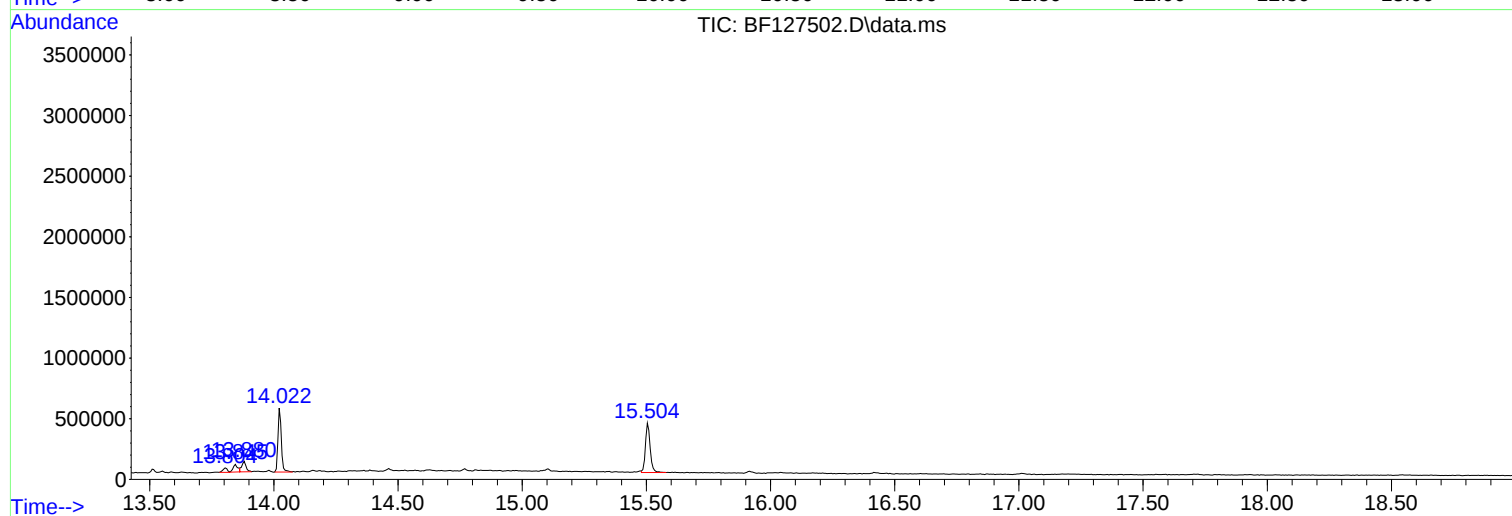
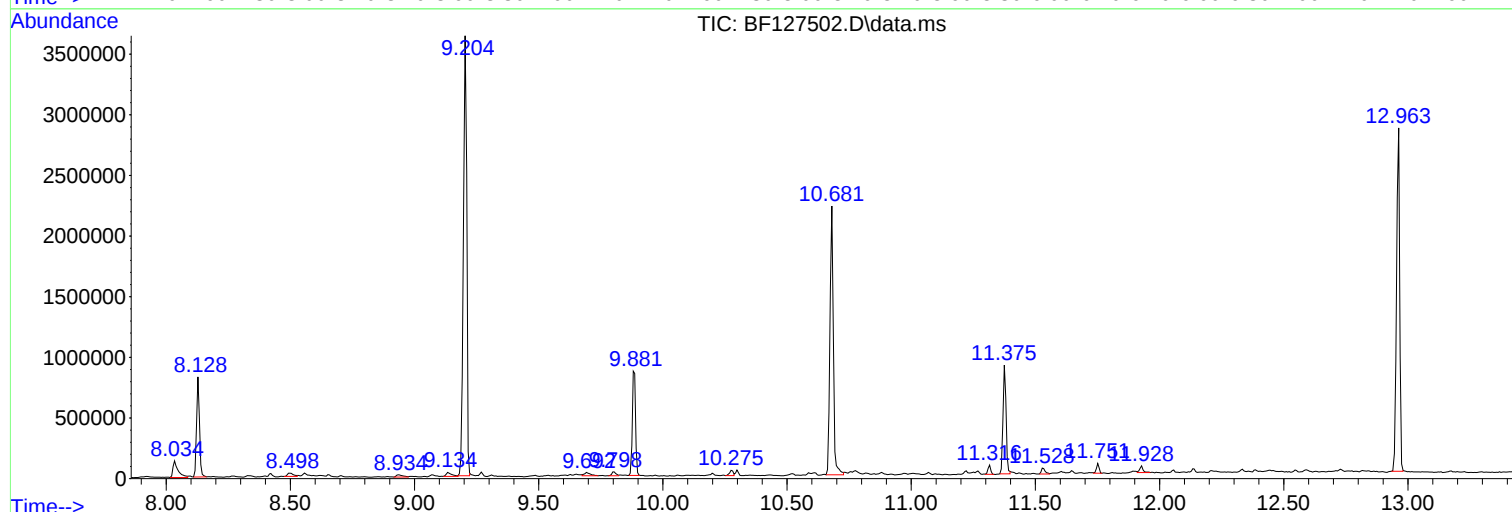
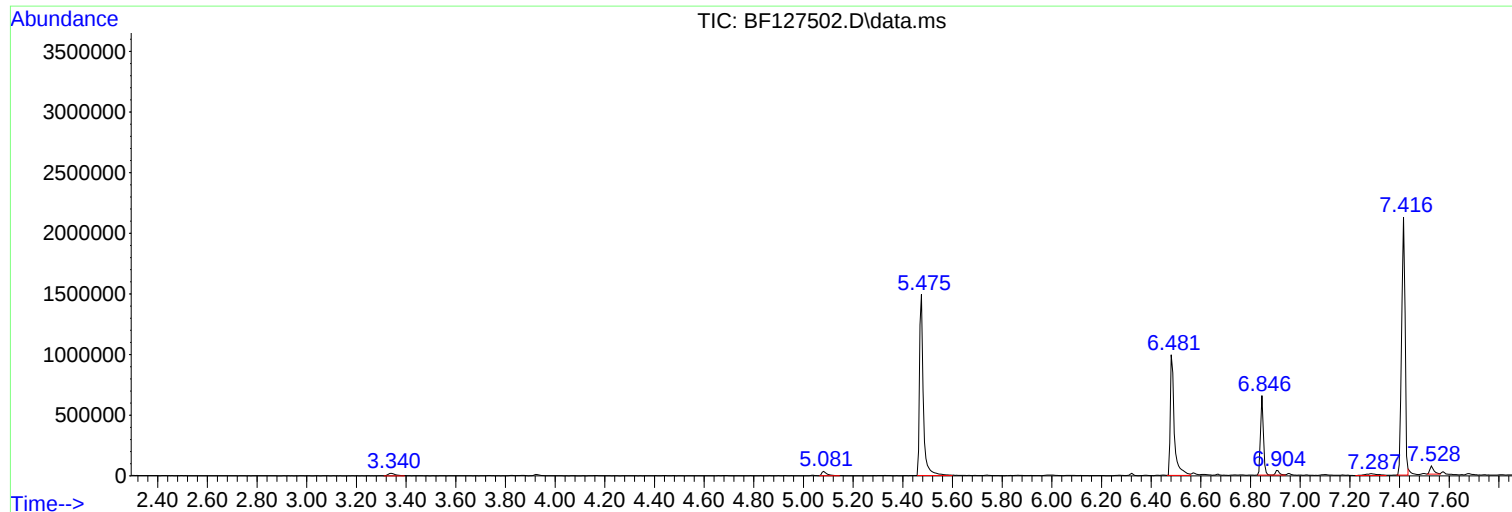
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Instrument :
BNA_F
ClientSampleId :
MW-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.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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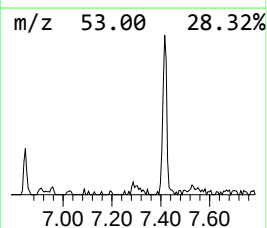
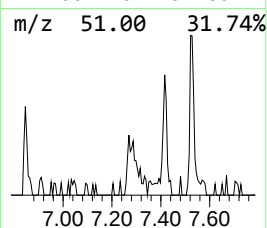
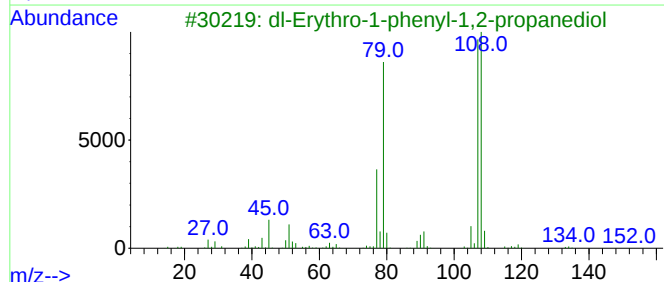
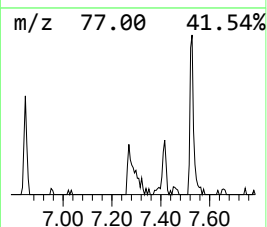
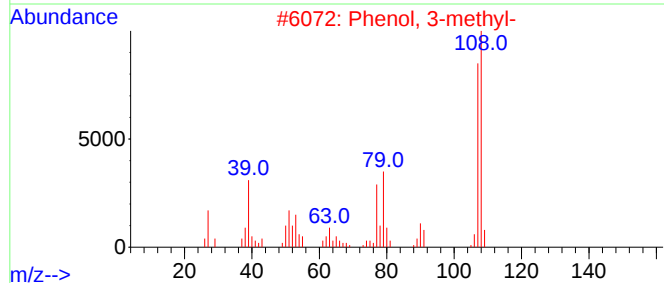
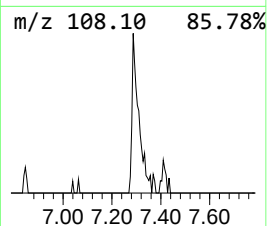
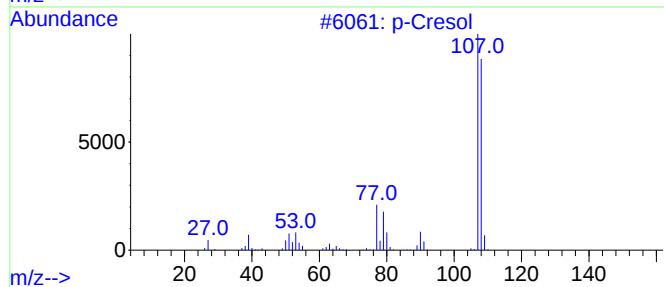
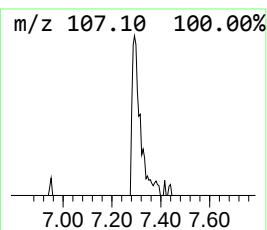
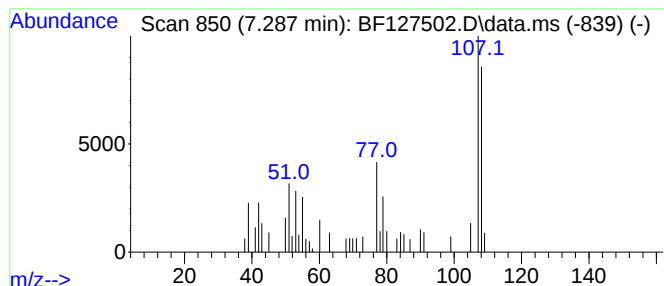
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 p-Cresol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.287	2.09 ng	55467	1,4-Dichlorobenzene-d4	6.846

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			p-Cresol	108	C7H8O	000106-44-5	90
2			Phenol, 3-methyl-	108	C7H8O	000108-39-4	74
3			dl-Erythro-1-phenyl-1,2-propanediol	152	C9H12O2	001075-04-3	59
4			Phenol, 2-methyl-	108	C7H8O	000095-48-7	58
5			1H-Imidazole, 1-methyl-2-vinyl-	108	C6H8N2	016975-71-6	47



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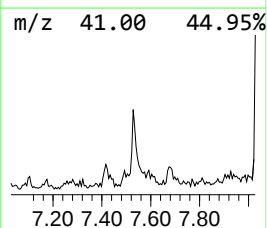
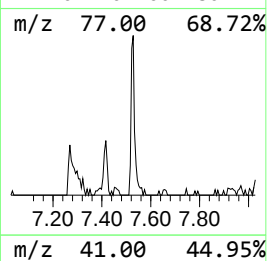
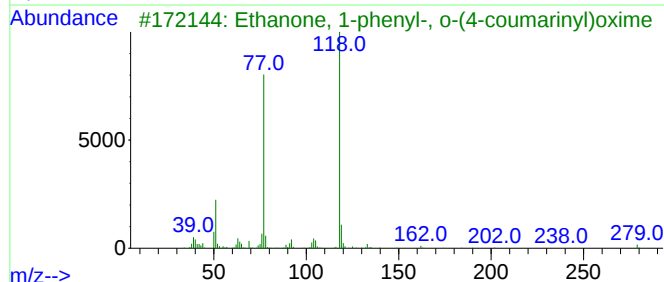
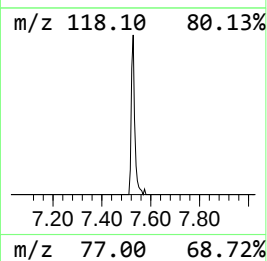
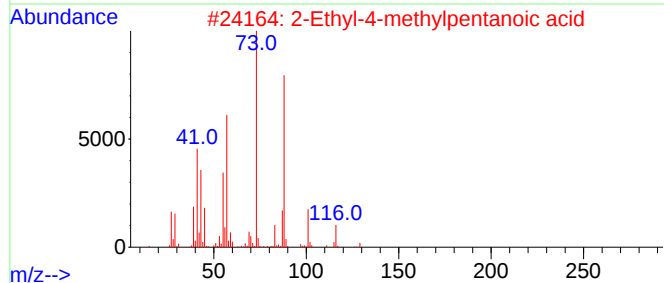
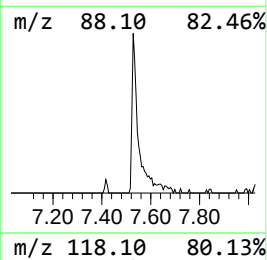
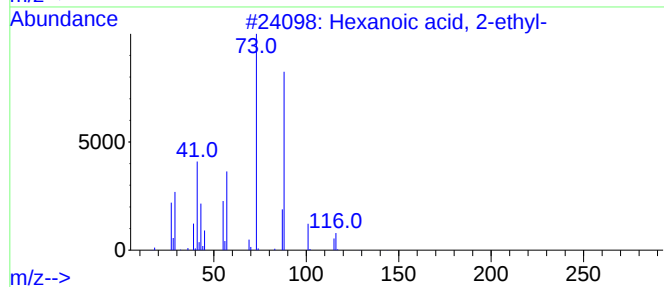
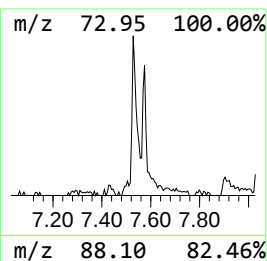
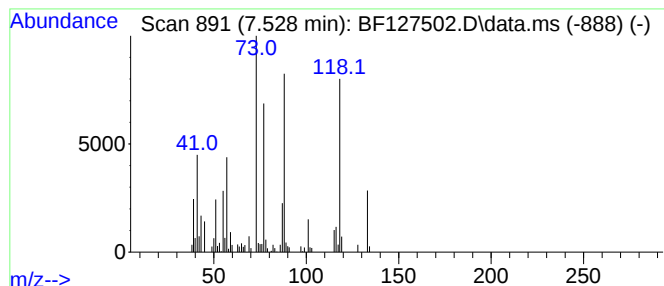
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown7.528 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.528	2.22 ng	75434	Naphthalene-d8	8.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	38
2			2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	35
3			Ethanone, 1-phenyl-, o-(4-coumar...	279	C17H13NO3	034605-11-3	27
4			Timonacic	133	C4H7NO2S	000444-27-9	22
5			Methanamine, N-(1-phenylethylide...	133	C9H11N	006907-71-7	16



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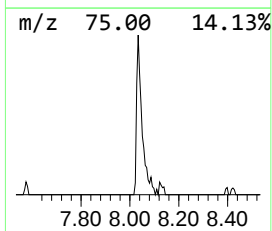
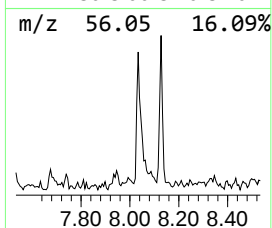
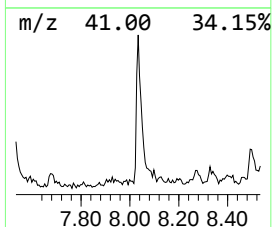
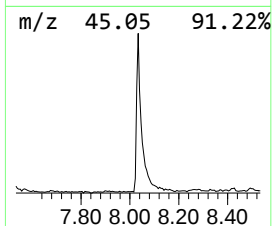
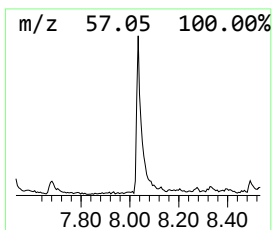
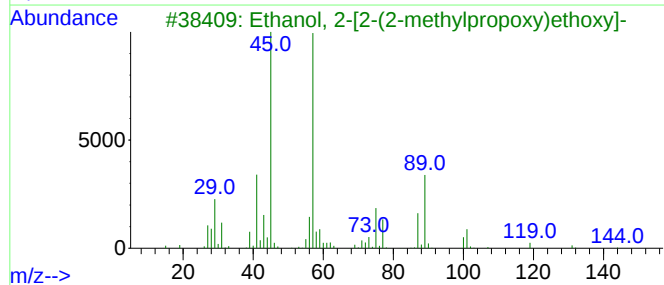
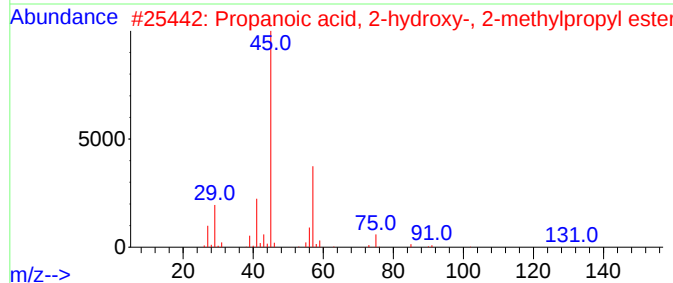
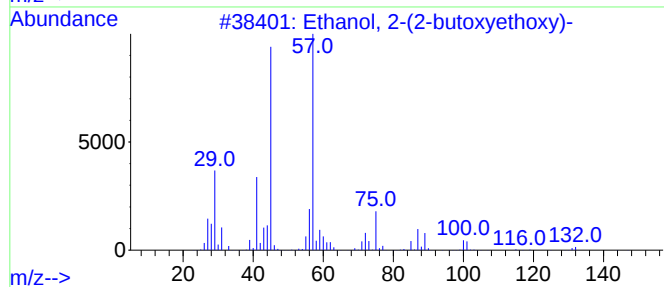
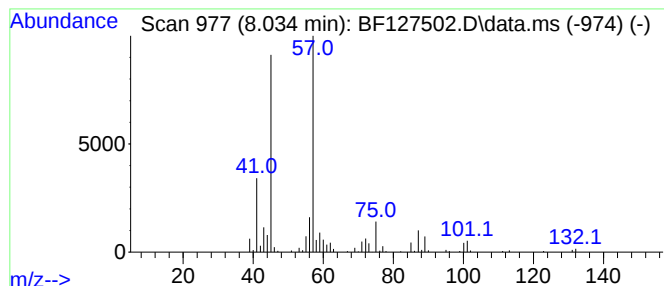
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.034	5.79 ng	196909	Naphthalene-d8	8.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	59
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5			Tetraethylene glycol	194	C8H18O5	000112-60-7	53



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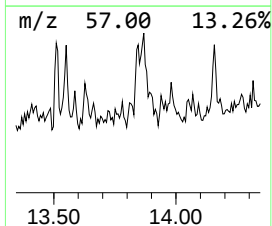
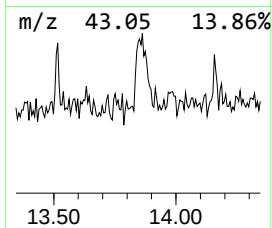
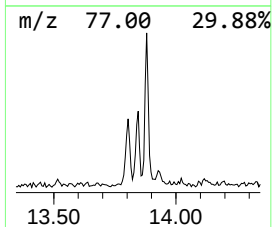
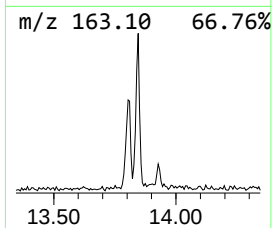
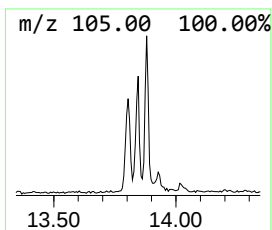
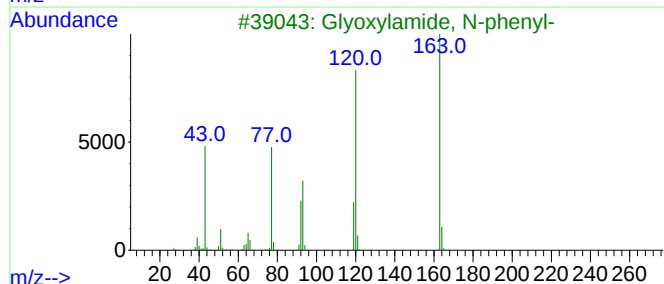
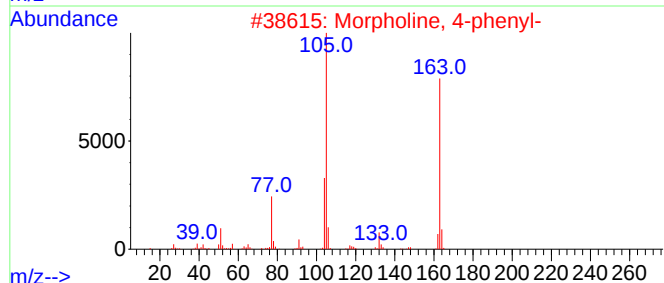
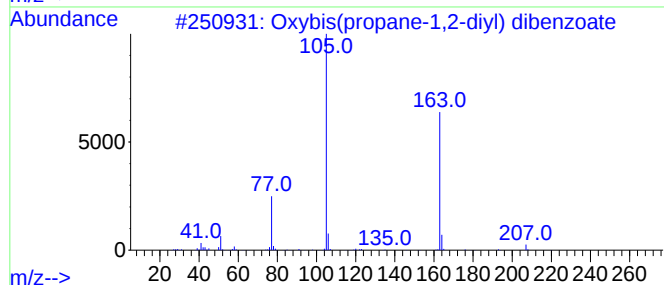
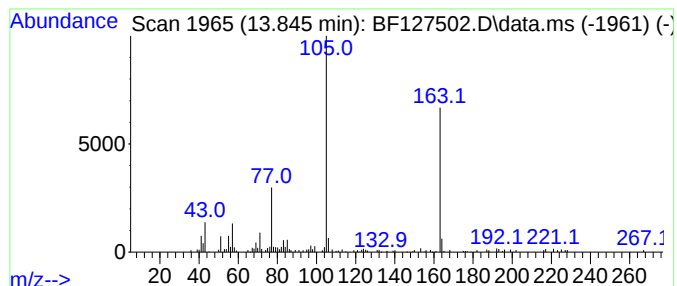
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Oxybis(propene-1,2-diyl) di... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	3.47 ng	87175	Chrysene-d12	14.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxybis(propene-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	59
2			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	43
3			Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	43
4			N-(4-Formyl-phenyl)-N-methyl-for...	163	C9H9NO2	079213-80-2	43
5			Benzoic acid, 3,3-dimethylbut-2-...	206	C13H18O2	1000368-20-7	27



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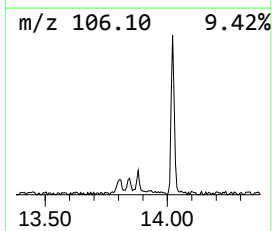
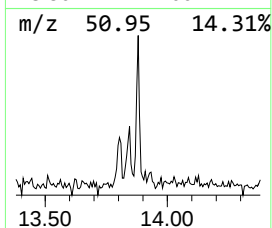
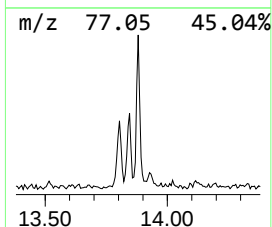
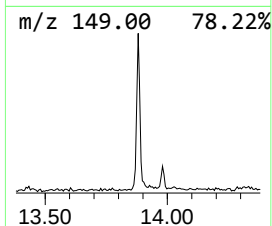
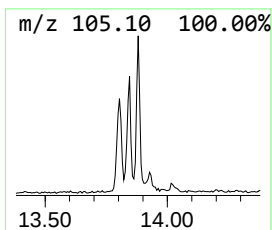
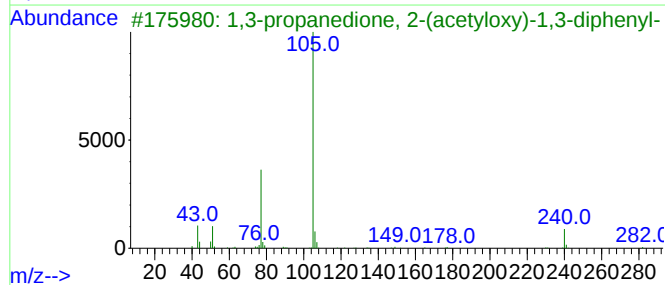
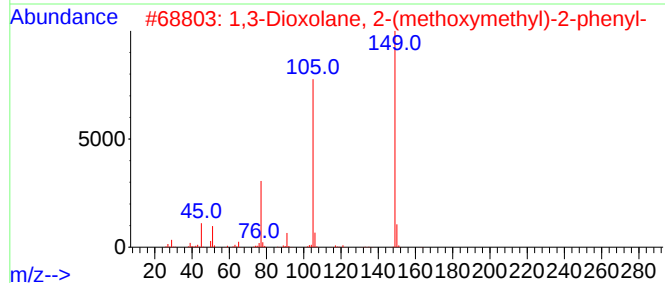
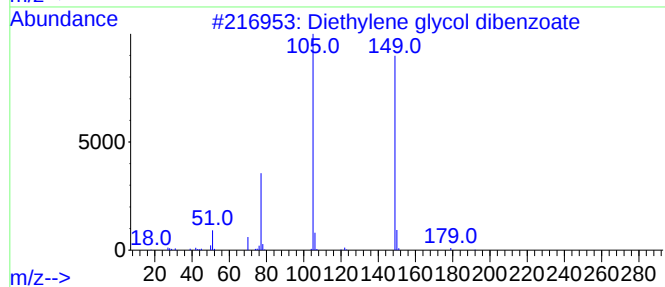
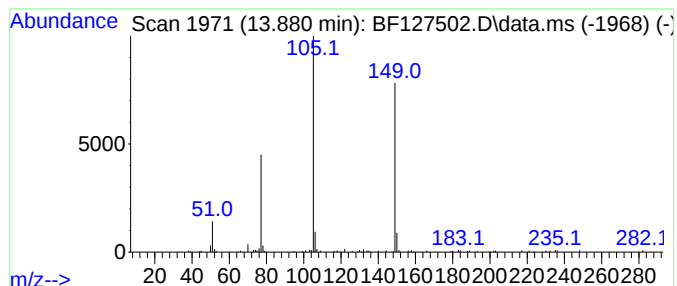
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Diethylene glycol dibenzoate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.880	4.06 ng	101980	Chrysene-d12	14.022	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2	1,3-Dioxolane, 2-(methoxymethyl)-...	194	C11H14O3	1000156-71-2	64
3	1,3-propanedione, 2-(acetyloxy)-...	282	C17H14O4	1000401-92-5	38
4	Benzamide, N-(3-ethynylphenyl)-	221	C15H11NO	208943-24-2	35
5	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	35



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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
p-Cresol	7.287	2.1	ng	55467	1	6.846	530373	20.0
unknown7.528	7.528	2.2	ng	75434	2	8.128	680204	20.0
Ethanol, 2-(2-b...	8.034	5.8	ng	196909	2	8.128	680204	20.0
Oxybis(propane-...	13.845	3.5	ng	87175	5	14.022	501778	20.0
Diethylene glyc...	13.880	4.1	ng	101980	5	14.022	501778	20.0