

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
 Data File : BF127174.D
 Acq On : 03 Mar 2022 16:39
 Operator : CG\JU
 Sample : N1689-04
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-40

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-BF021622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127174.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.034	122	127	136	rVB3	22676	40472	1.25%	0.177%
2	3.240	155	162	167	rBV	157607	274715	8.49%	1.200%
3	4.416	357	362	366	rBV	118446	141039	4.36%	0.616%
4	4.504	372	377	381	rVB2	172217	197135	6.09%	0.861%
5	5.510	544	548	558	rVB	1353709	1190621	36.80%	5.203%
6	5.928	611	619	625	rBV7	21834	48129	1.49%	0.210%
7	6.486	709	714	716	rBV3	33906	37116	1.15%	0.162%
8	6.516	716	719	724	rVV	877204	789535	24.40%	3.450%
9	6.569	724	728	730	rVB2	26755	38267	1.18%	0.167%
10	6.710	741	752	759	rBV2	80839	144709	4.47%	0.632%
11	6.886	778	782	786	rBV	623861	515875	15.95%	2.254%
12	6.945	789	792	795	rVV2	83318	69413	2.15%	0.303%
13	7.034	798	807	809	rBV	78671	104060	3.22%	0.455%
14	7.086	809	816	819	rVV3	114665	310335	9.59%	1.356%
15	7.157	821	828	831	rVV	194707	425288	13.15%	1.858%
16	7.210	833	837	841	rBV4	46477	53021	1.64%	0.232%
17	7.457	862	879	881	rBV	2108375	2544781	78.66%	11.120%
18	7.486	881	884	888	rVV3	493807	1052474	32.53%	4.599%
19	7.528	888	891	895	rVB3	568608	832205	25.72%	3.637%
20	7.739	922	927	932	rVB	228996	237761	7.35%	1.039%
21	7.904	950	955	964	rBV8	40400	71357	2.21%	0.312%
22	7.992	964	970	972	rBV3	44155	58677	1.81%	0.256%
23	8.098	985	988	994	rVB5	60668	92572	2.86%	0.405%
24	8.169	994	1000	1004	rBV	766225	716935	22.16%	3.133%
25	8.292	1016	1021	1028	rBV9	25405	45571	1.41%	0.199%
26	8.363	1028	1033	1036	rBV6	34251	52964	1.64%	0.231%
27	8.433	1036	1045	1048	rBV7	36599	71820	2.22%	0.314%
28	8.533	1057	1062	1066	rBV7	29346	48548	1.50%	0.212%
29	8.628	1075	1078	1081	rBV3	59807	50267	1.55%	0.220%
30	8.986	1135	1139	1141	rBV3	90264	122864	3.80%	0.537%
31	9.022	1141	1145	1147	rVV2	139292	228559	7.06%	0.999%
32	9.051	1148	1150	1156	rVV2	157851	181457	5.61%	0.793%
33	9.110	1156	1160	1165	rVV2	84615	106181	3.28%	0.464%
34	9.163	1165	1169	1174	rVB3	77989	88472	2.73%	0.387%
35	9.251	1179	1184	1187	rBV	3752277	3235229	100.00%	14.137%
36	9.439	1212	1216	1222	rBV	188534	191899	5.93%	0.839%

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37	9.498	1222	1226	1229	rBV	64465	68097	2.10%	0.298%
38	9.545	1229	1234	1237	rBV2	110857	135187	4.18%	0.591%
39	9.669	1252	1255	1258	rBV	67424	65958	2.04%	0.288%
40	9.745	1265	1268	1271	rVB2	141505	128117	3.96%	0.560%
41	9.798	1271	1277	1279	rVV4	58237	85184	2.63%	0.372%
42	9.845	1281	1285	1289	rVB	144713	166094	5.13%	0.726%
43	9.933	1296	1300	1303	rBV	826145	765933	23.67%	3.347%
44	10.192	1339	1344	1347	rBV4	40613	64441	1.99%	0.282%
45	10.327	1362	1367	1369	rBV2	39070	54339	1.68%	0.237%
46	10.727	1430	1435	1438	rBV	2315064	2160388	66.78%	9.440%
47	11.298	1530	1532	1536	rVB4	35589	39624	1.22%	0.173%
48	11.363	1540	1543	1548	rVB2	74757	69028	2.13%	0.302%
49	11.421	1549	1553	1556	rBV	913170	731301	22.60%	3.196%
50	11.580	1577	1580	1585	rBV	46795	48836	1.51%	0.213%
51	11.939	1638	1641	1645	rBV	86795	78101	2.41%	0.341%
52	11.974	1645	1647	1650	rVB	53545	43446	1.34%	0.190%
53	13.010	1818	1823	1826	rBV	3177565	2866740	88.61%	12.527%
54	13.933	1977	1980	1981	rBV	37870	40694	1.26%	0.178%
55	14.068	1999	2003	2006	rBV	460484	428295	13.24%	1.872%
56	15.556	2251	2256	2264	rBV	335108	434157	13.42%	1.897%

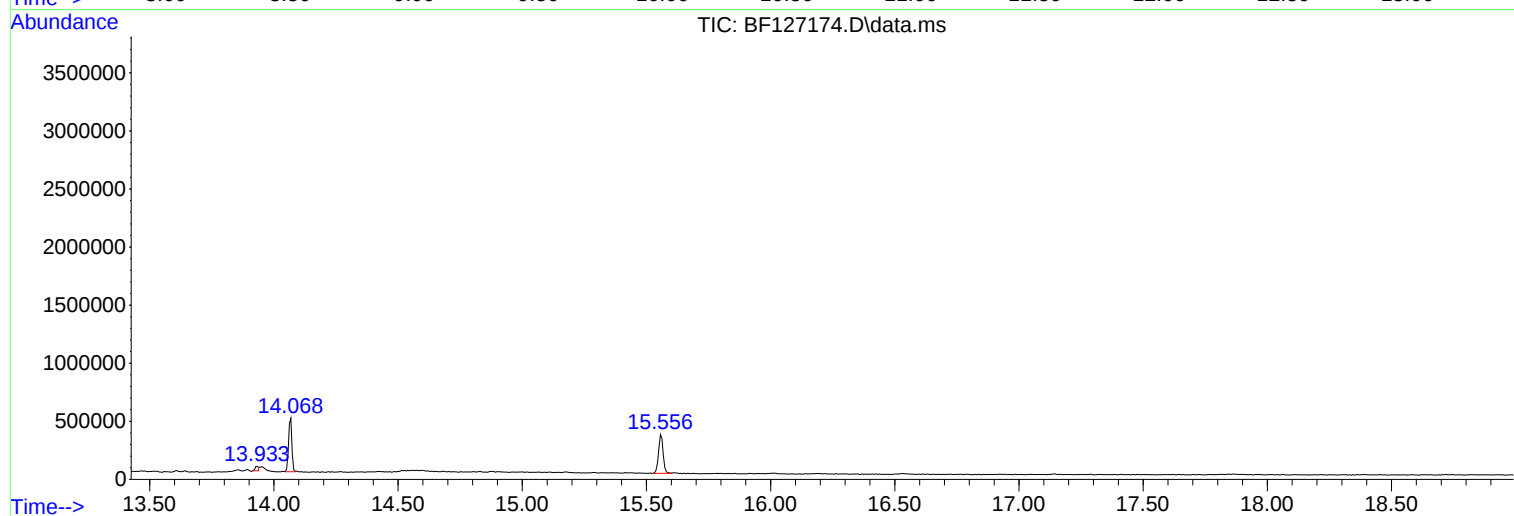
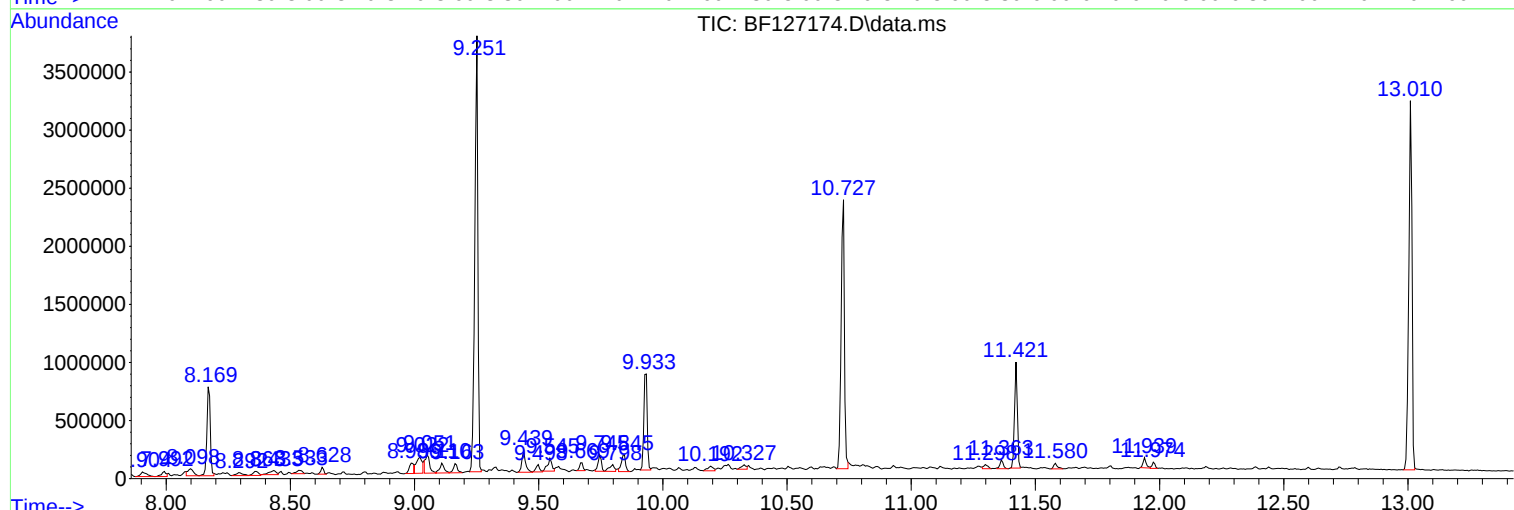
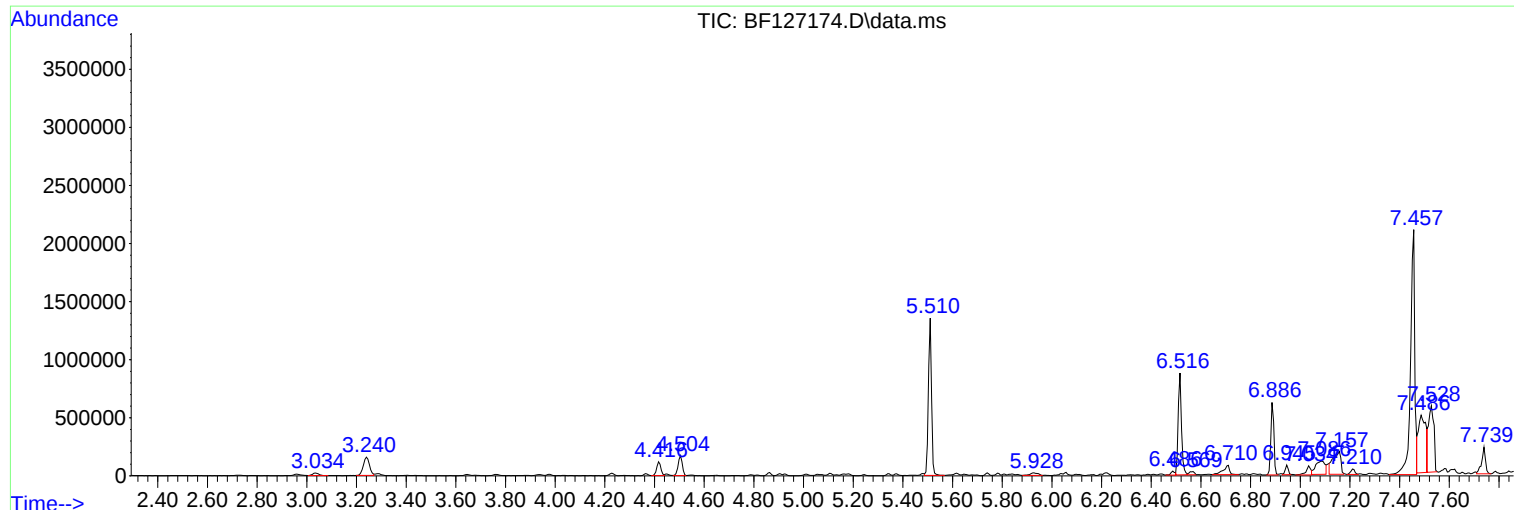
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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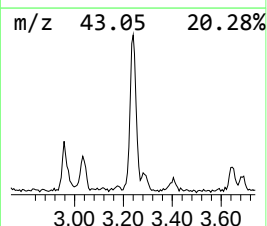
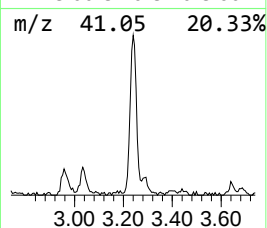
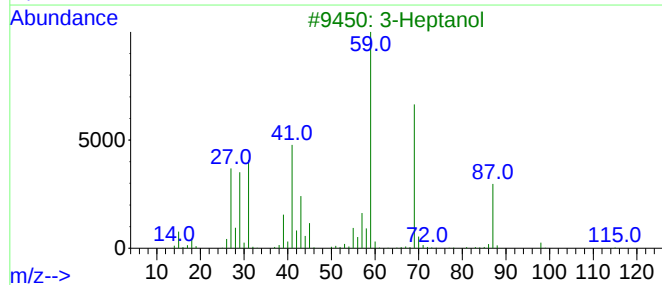
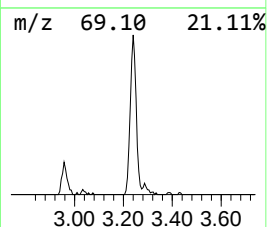
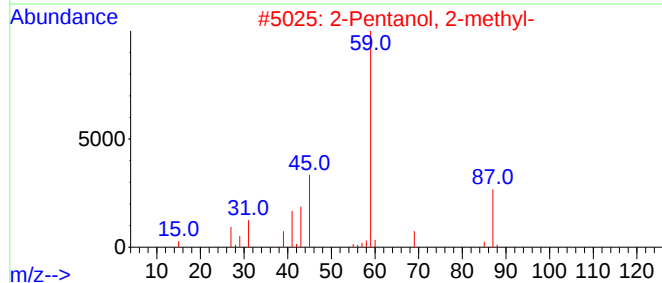
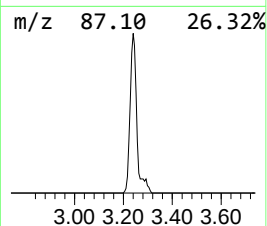
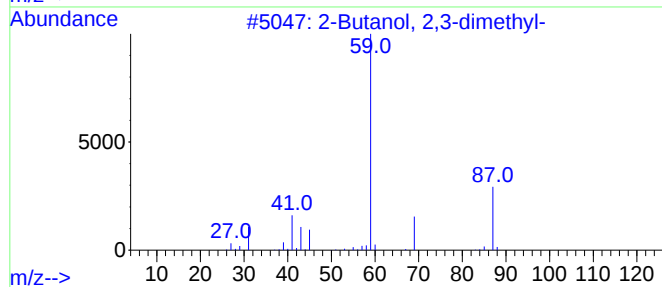
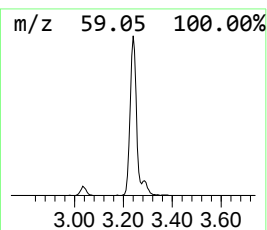
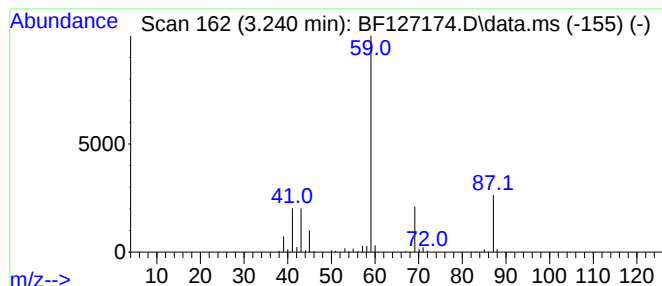
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Butanol, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.240	10.65 ng	274715	1,4-Dichlorobenzene-d4	6.886

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	83
2		2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	72
3		3-Heptanol	116	C7H16O	000589-82-2	40
4		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	39
5		2-Decanol, methyl ether	172	C11H24O	1000333-83-9	36



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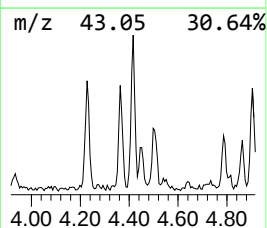
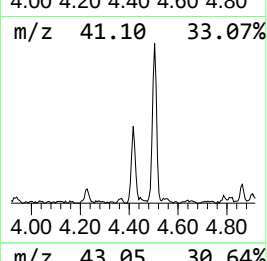
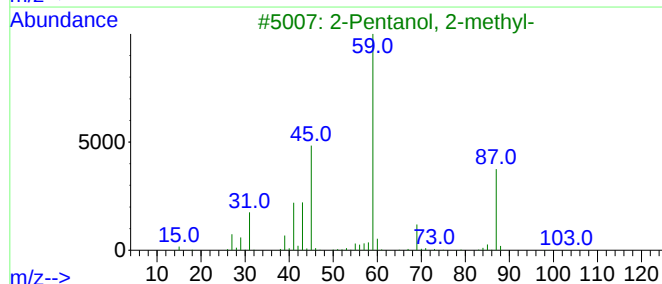
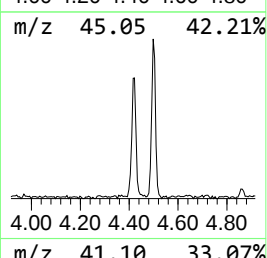
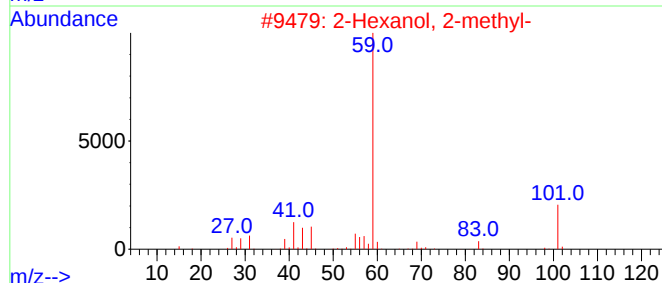
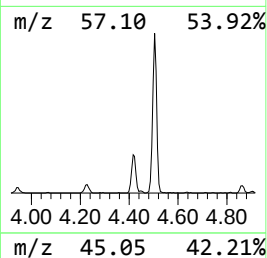
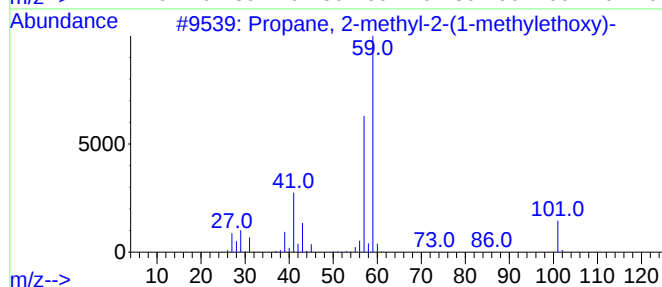
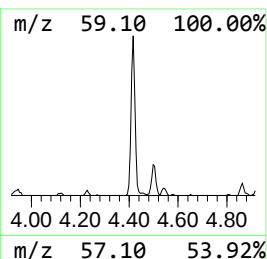
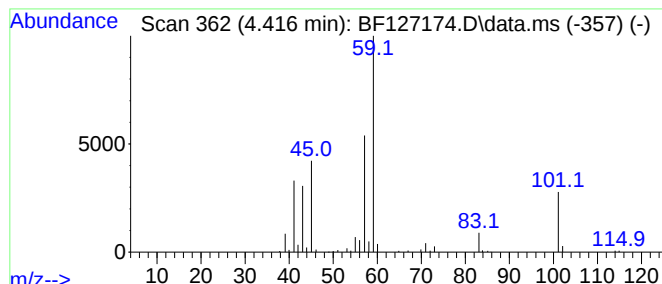
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 2-methyl-2-(1-meth... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.416	5.47 ng	141039	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	45
3			2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	45
4			Hexanamide	115	C6H13NO	000628-02-4	43
5			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	42



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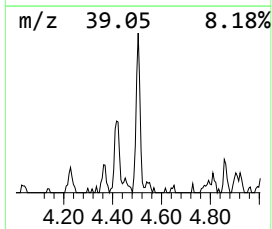
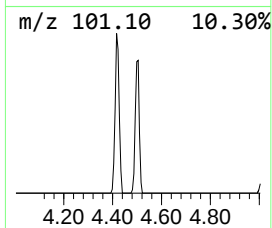
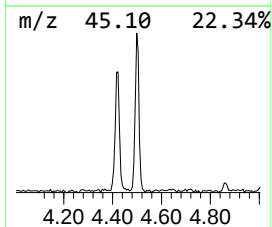
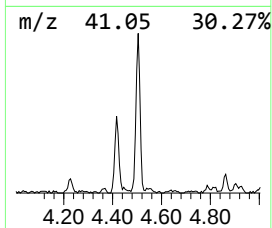
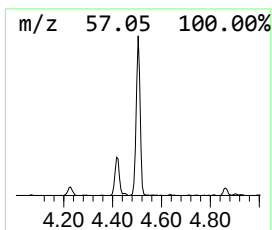
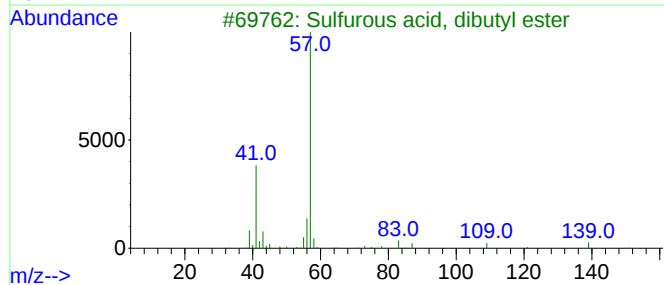
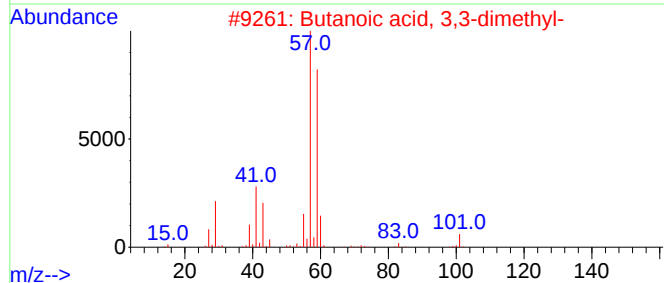
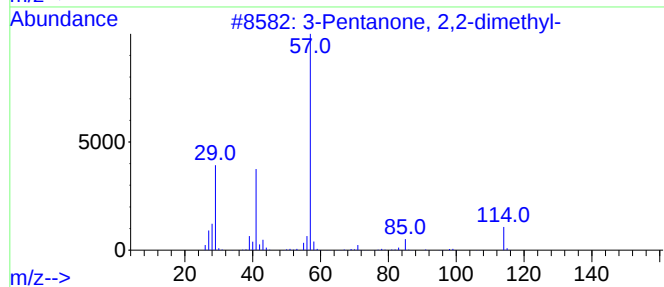
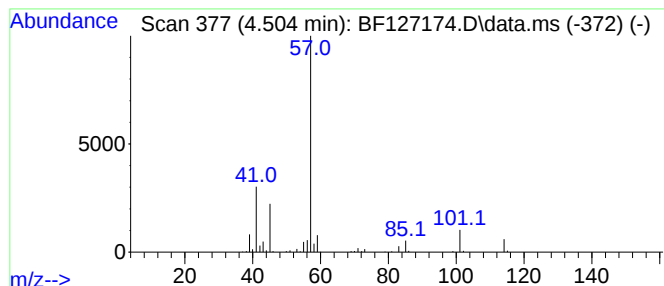
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown4.504 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.504	7.64 ng	197135	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone, 2,2-dimethyl-	114	C7H14O	000564-04-5	43
2			Butanoic acid, 3,3-dimethyl-	116	C6H12O2	001070-83-3	32
3			Sulfurous acid, dibutyl ester	194	C8H18O3S	000626-85-7	27
4			Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	25
5			Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	23



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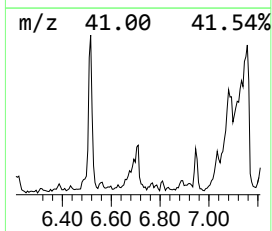
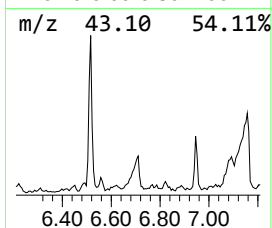
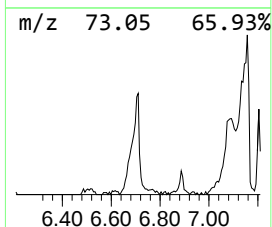
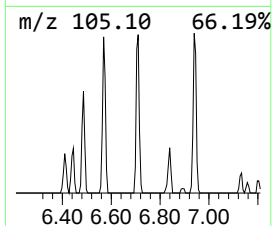
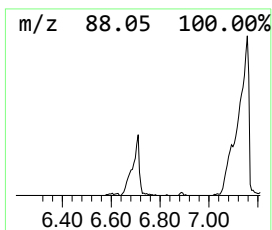
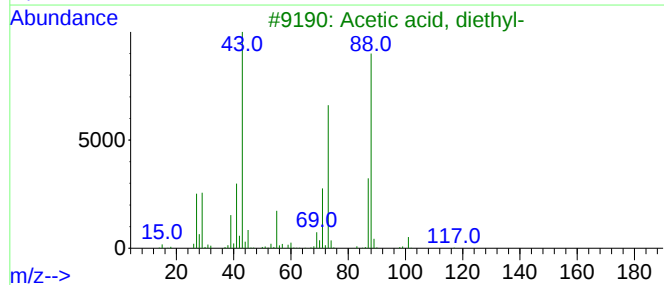
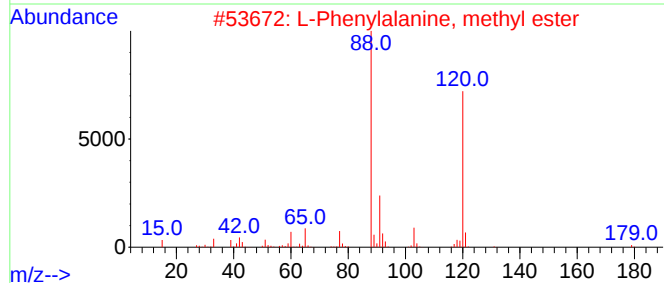
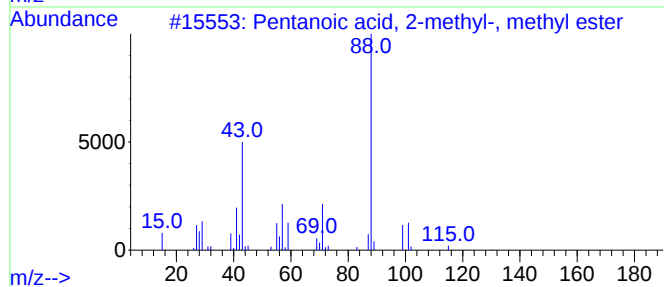
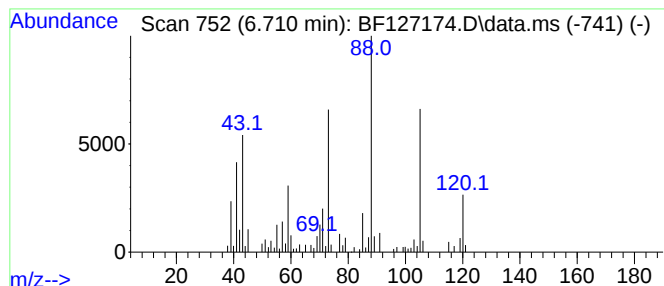
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown6.710 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.710	5.61 ng	144709	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanoic acid, 2-methyl-, methy...	130	C7H14O2	002177-77-7	47
2			L-Phenylalanine, methyl ester	179	C10H13NO2	002577-90-4	43
3			Acetic acid, diethyl-	116	C6H12O2	000088-09-5	38
4			Sulfide, allyl methyl	88	C4H8S	010152-76-8	38
5			Urea, ethyl-	88	C3H8N2O	000625-52-5	35



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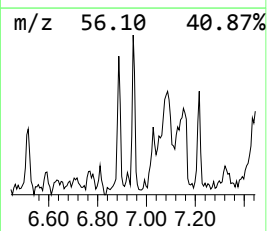
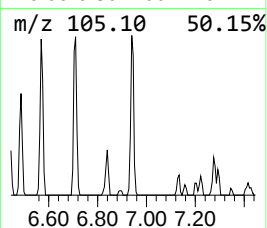
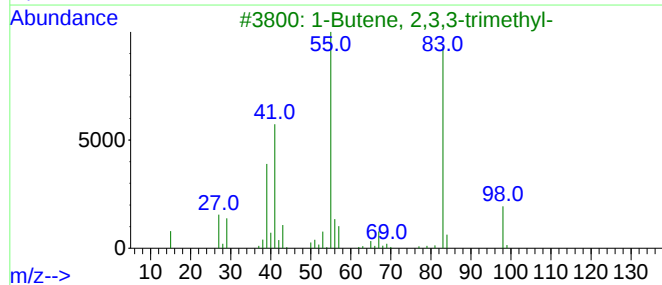
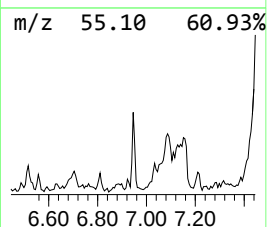
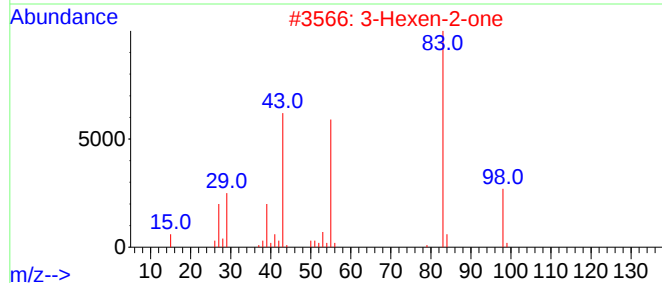
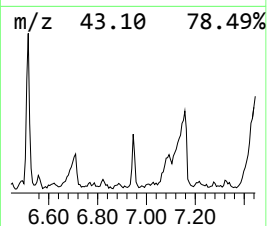
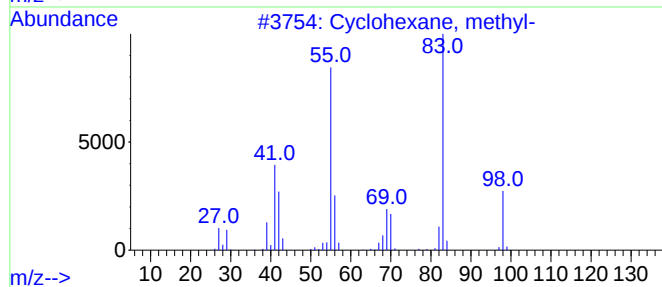
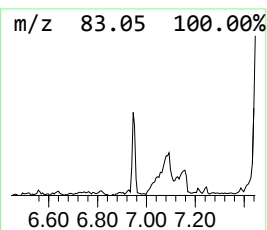
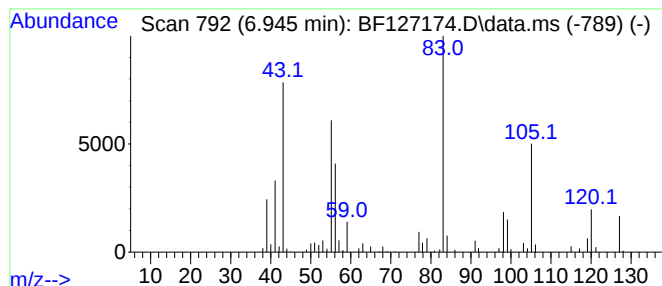
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown6.945 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.945	2.69 ng	69413	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, methyl-	98	C7H14	000108-87-2	43
2			3-Hexen-2-one	98	C6H10O	000763-93-9	38
3			1-Butene, 2,3,3-trimethyl-	98	C7H14	000594-56-9	35
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	35
5			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
Data File : BF127174.D
Acq On : 03 Mar 2022 16:39
Operator : CG\JU
Sample : N1689-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

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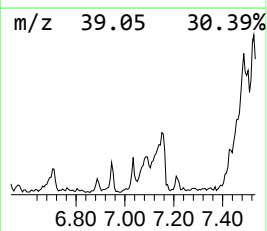
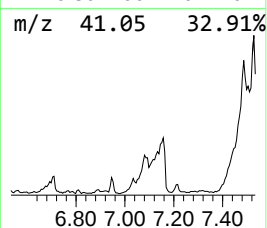
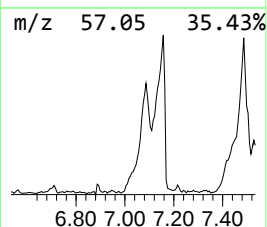
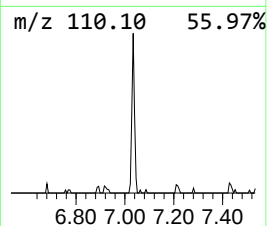
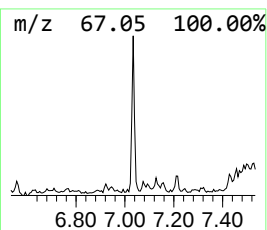
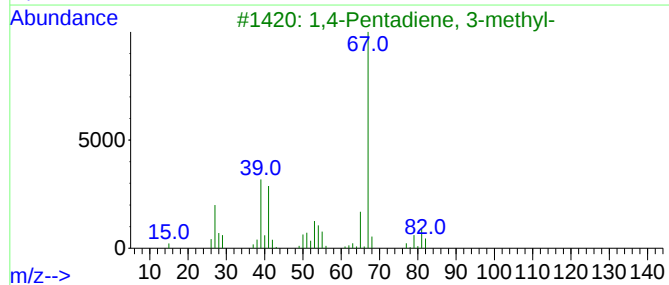
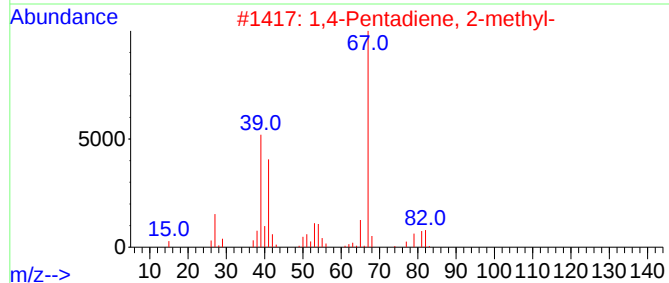
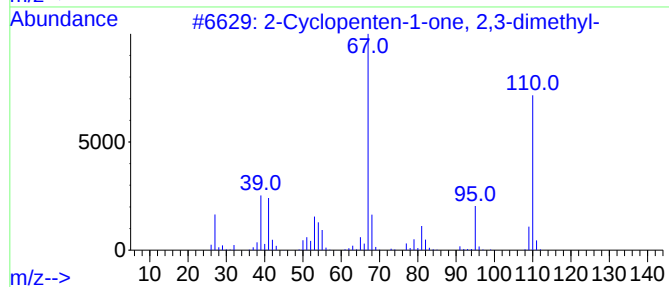
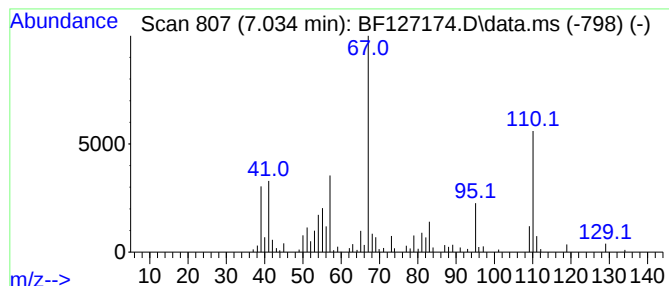
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-Cyclopenten-1-one, 2,3-di... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.034	4.03 ng	104060	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclopenten-1-one, 2,3-dimethyl-	110	C7H10O	001121-05-7	81
2			1,4-Pentadiene, 2-methyl-	82	C6H10	000763-30-4	30
3			1,4-Pentadiene, 3-methyl-	82	C6H10	001115-08-8	30
4			1H-Pyrazole, 1,3,5-trimethyl-	110	C6H10N2	001072-91-9	30
5			Cyclopentene, 3-methyl-	82	C6H10	001120-62-3	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
Data File : BF127174.D
Acq On : 03 Mar 2022 16:39
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Sample : N1689-04
Misc :
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Instrument :
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ClientSampleId :
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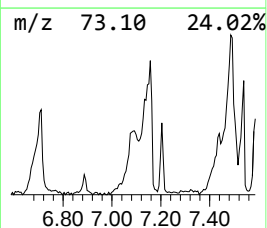
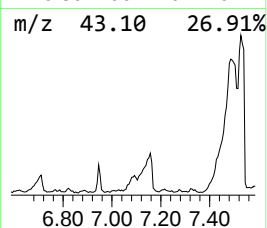
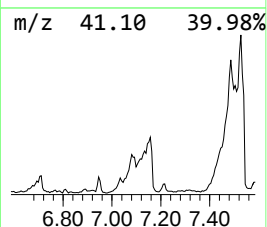
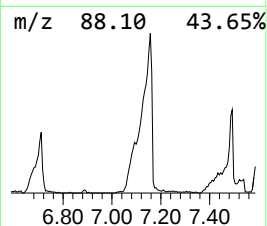
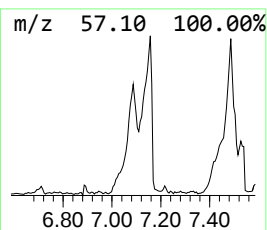
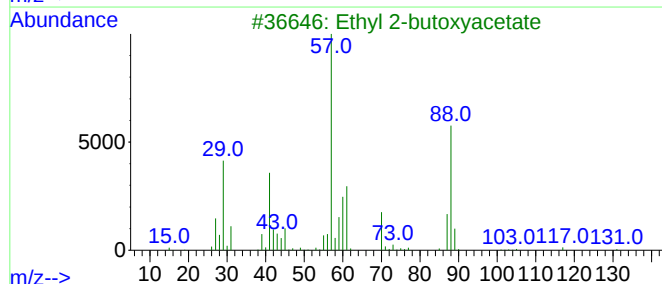
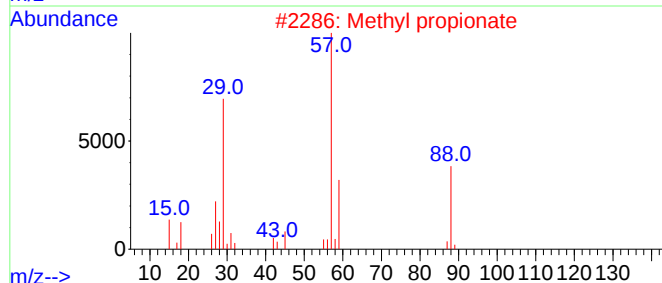
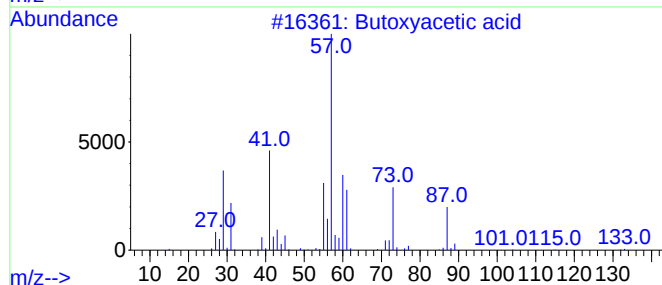
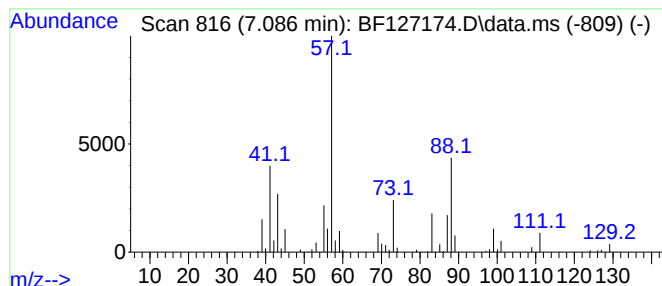
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown7.086 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.086	12.03 ng	310335	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butoxyacetic acid	132	C6H12O3	002516-93-0	35
2			Methyl propionate	88	C4H8O2	000554-12-1	32
3			Ethyl 2-butoxyacetate	160	C8H16O3	1000366-89-3	28
4			Sulfurous acid, 2-propyl heptyl ...	222	C10H22O3S	1000309-11-8	27
5			Propanoic acid, 2,2-dimethyl-, m...	116	C6H12O2	000598-98-1	16



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
Data File : BF127174.D
Acq On : 03 Mar 2022 16:39
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Sample : N1689-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

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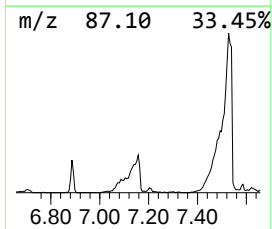
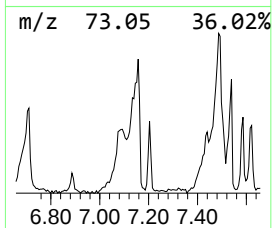
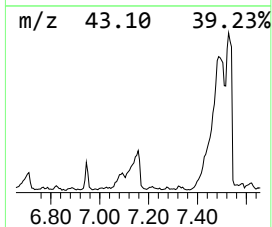
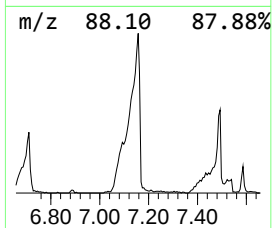
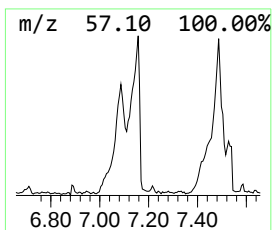
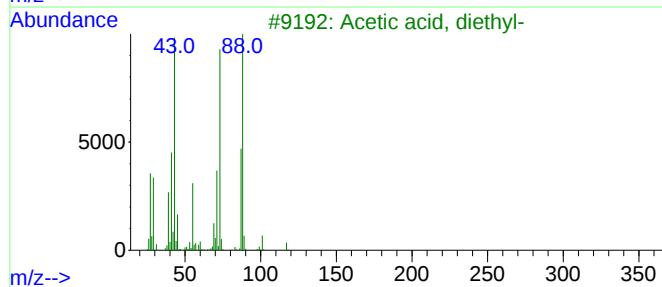
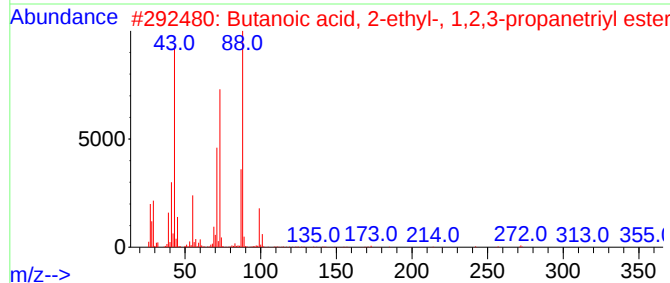
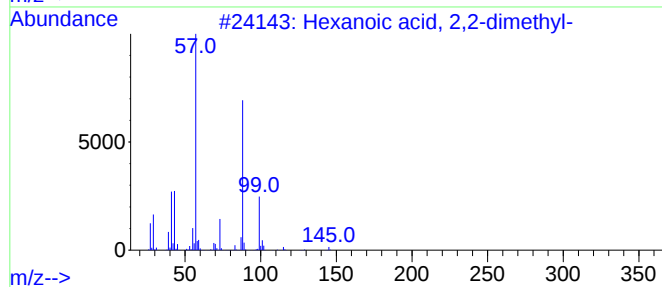
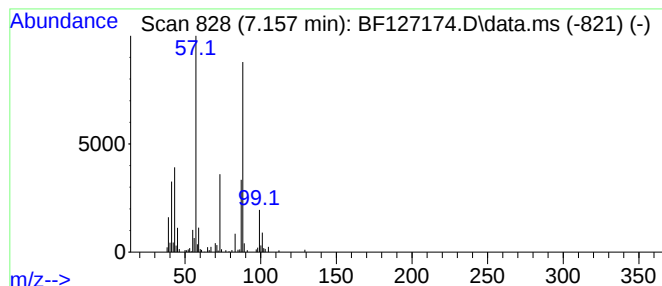
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexanoic acid, 2,2-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.157	16.49 ng	425288	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2,2-dimethyl-	144	C8H16O2	000813-72-9	59
2			Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	50
3			Acetic acid, diethyl-	116	C6H12O2	000088-09-5	50
4			Butyric acid, 2,2,3,3-tetramethyl-	144	C8H16O2	030407-41-1	40
5			Methyl-4-deoxy-2,3-di-O-methyl.b...	218	C9H14O6	1000312-09-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
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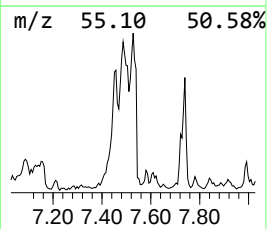
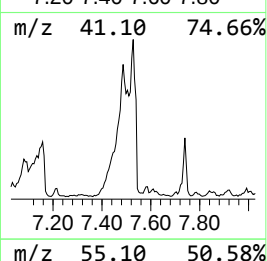
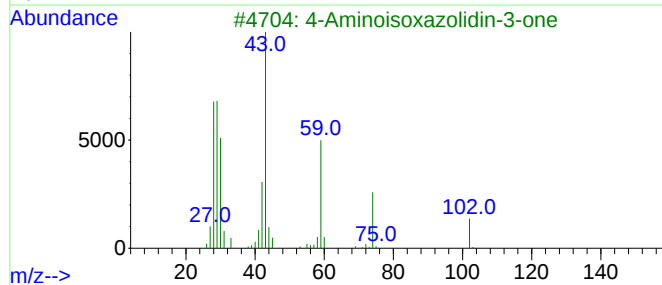
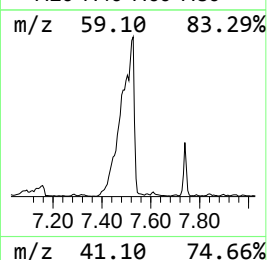
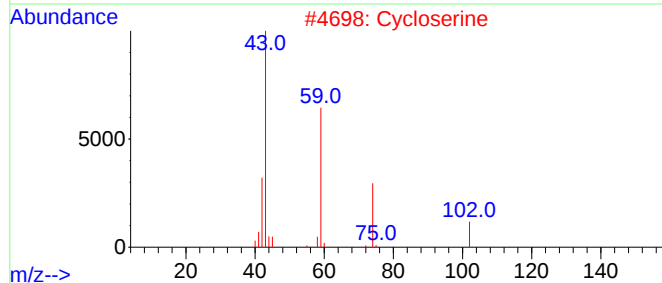
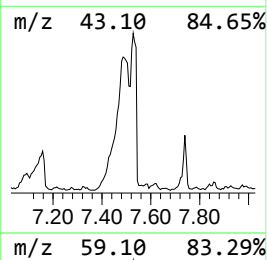
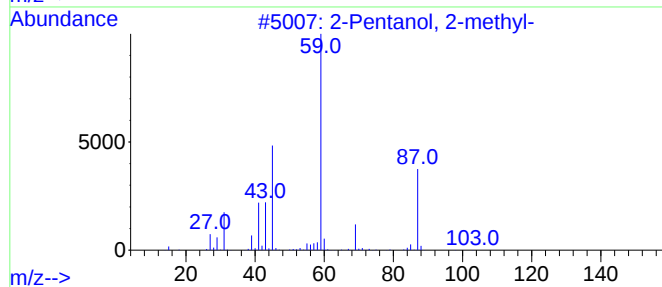
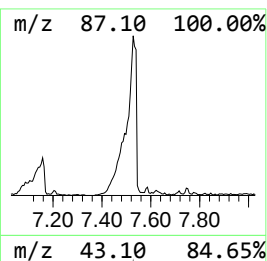
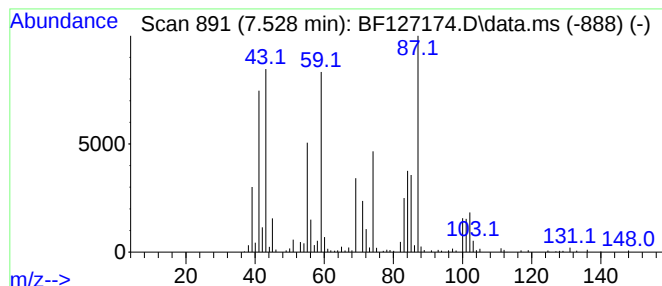
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown7.528 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.528	23.22 ng	832205	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 2-methyl-			102	C6H14O	000590-36-3	37
2	Cycloserine			102	C3H6N2O2	000068-41-7	27
3	4-Aminoisoxazolidin-3-one			102	C3H6N2O2	004834-58-6	25
4	1,3-Propanediol, 2,2-diethyl-			132	C7H16O2	000115-76-4	25
5	Ethane, isothiocyanato-			87	C3H5NS	000542-85-8	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
Data File : BF127174.D
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Misc :
ALS Vial : 5 Sample Multiplier: 1

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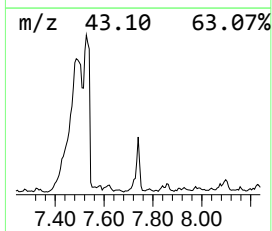
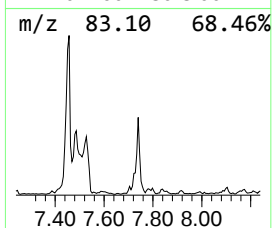
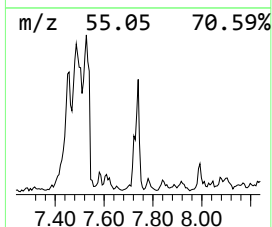
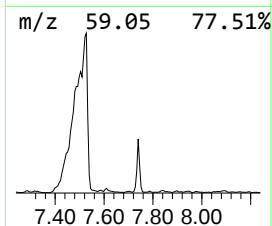
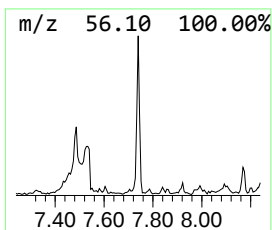
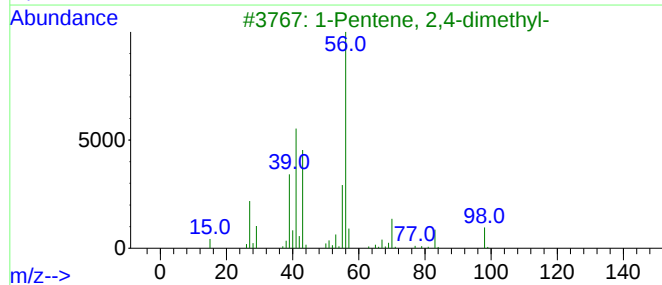
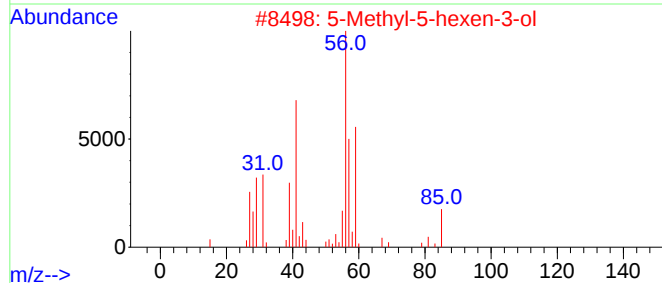
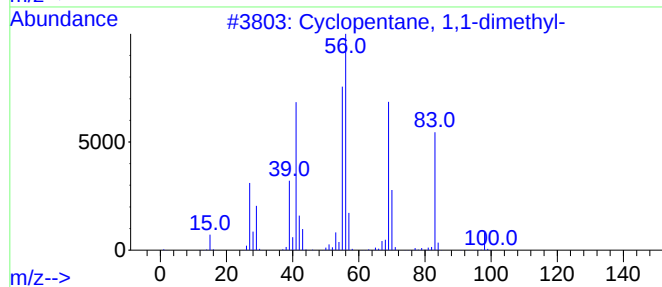
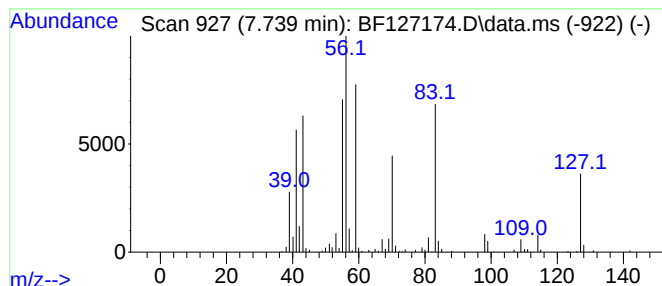
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown7.739 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.739	6.63 ng	237761	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	43
2			5-Methyl-5-hexen-3-ol	114	C7H14O	067760-89-8	43
3			1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	25
4			3,3-Dimethylpyrrolidine-2,5-dione	127	C6H9NO2	003437-29-4	22
5			2-Heptene, (E)-	98	C7H14	014686-13-6	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
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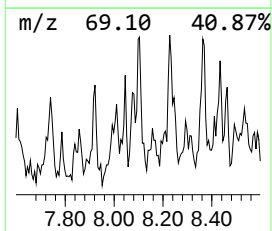
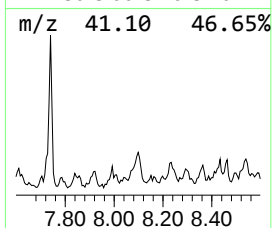
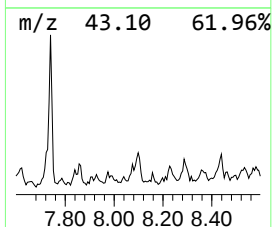
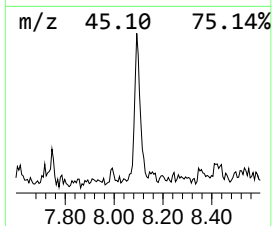
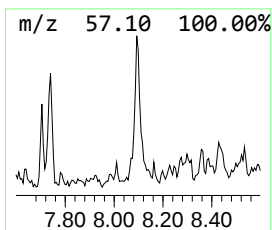
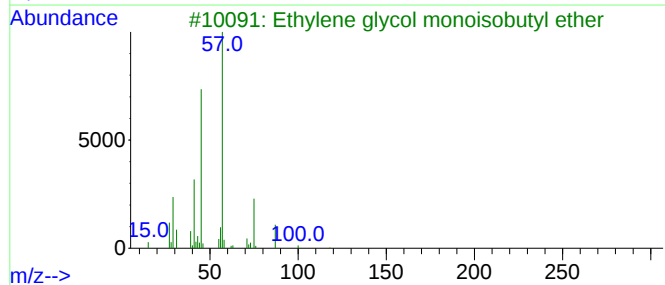
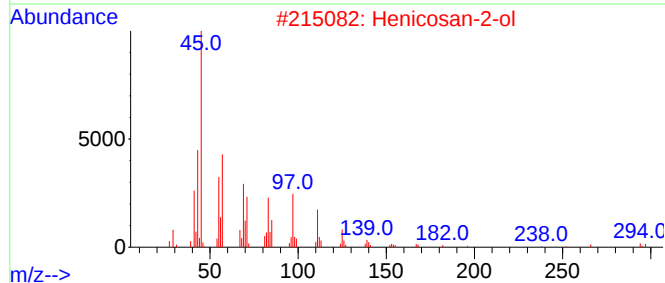
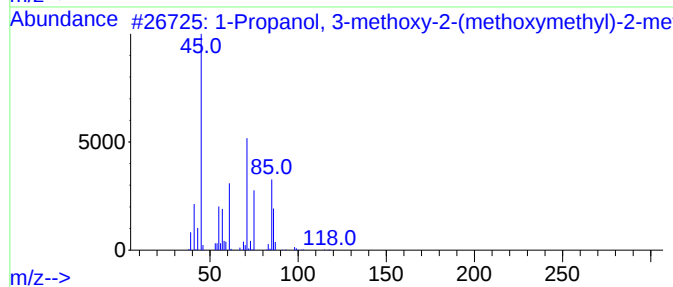
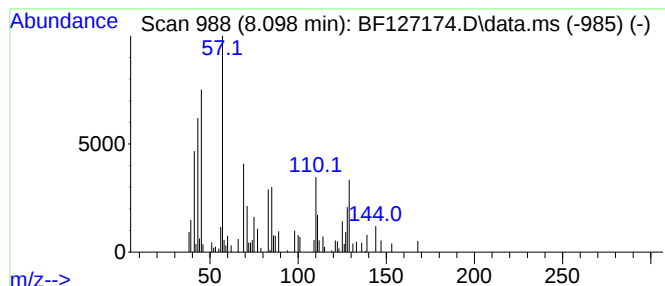
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown8.098 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	2.58 ng	92572	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 3-methoxy-2-(methoxy...	148	C7H16O3	020637-34-7	35		
2	Henicosan-2-ol	312	C21H44O	121232-91-5	32		
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	27		
4	Tetraethylene glycol	194	C8H18O5	000112-60-7	27		
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	27		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
Data File : BF127174.D
Acq On : 03 Mar 2022 16:39
Operator : CG\JU
Sample : N1689-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-40

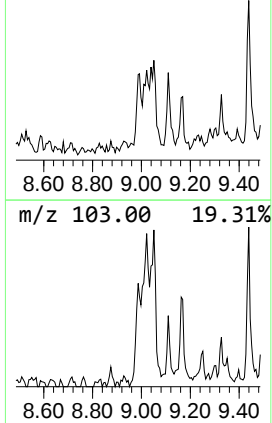
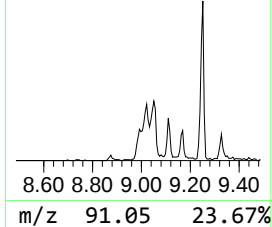
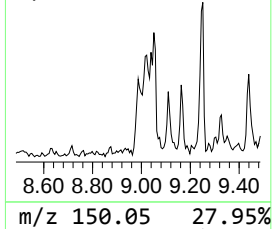
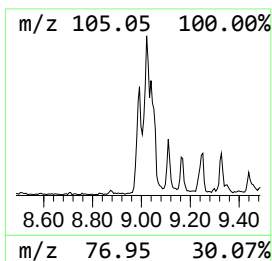
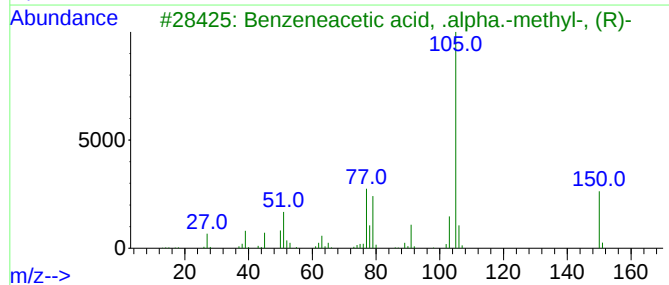
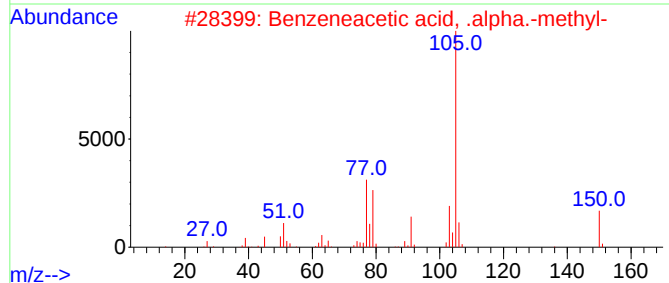
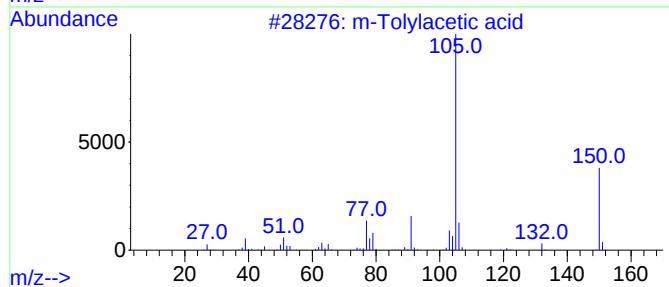
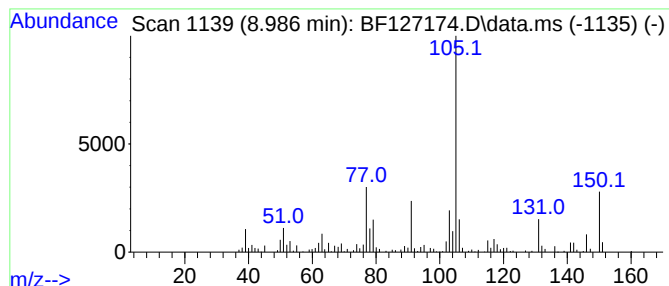
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 m-Tolylacetic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.986	3.43 ng	122864	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			m-Tolylacetic acid	150	C9H10O2	000621-36-3	90
2			Benzeneacetic acid, .alpha.-methyl-	150	C9H10O2	000492-37-5	81
3			Benzeneacetic acid, .alpha.-meth...	150	C9H10O2	007782-26-5	76
4			Benzeneacetic acid, .alpha.-meth...	150	C9H10O2	007782-24-3	76
5			o-Tolylacetic acid	150	C9H10O2	000644-36-0	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
Data File : BF127174.D
Acq On : 03 Mar 2022 16:39
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Sample : N1689-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

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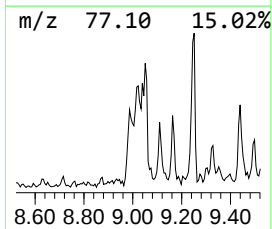
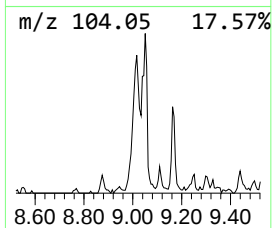
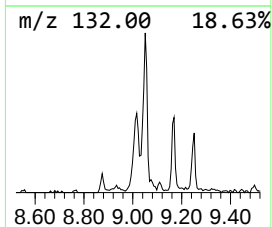
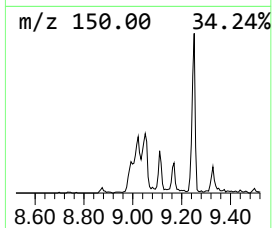
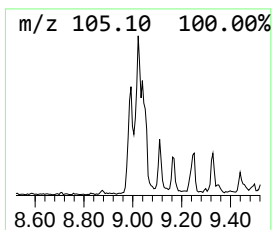
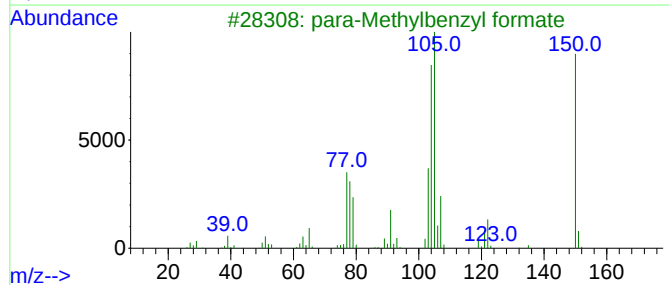
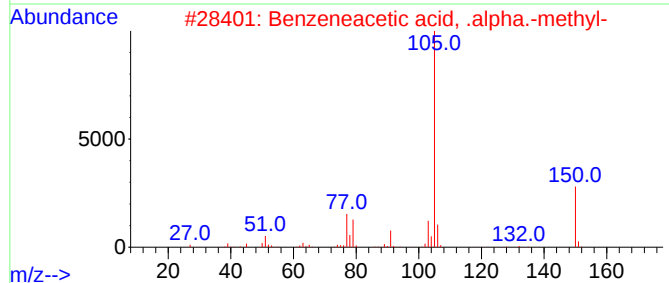
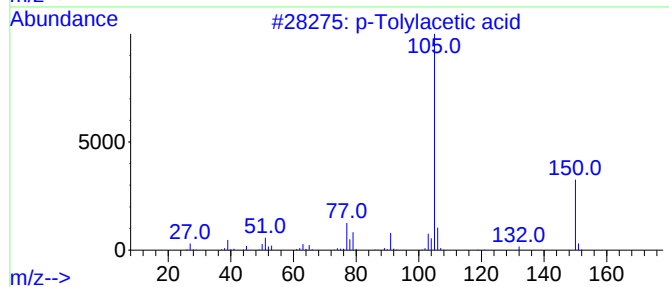
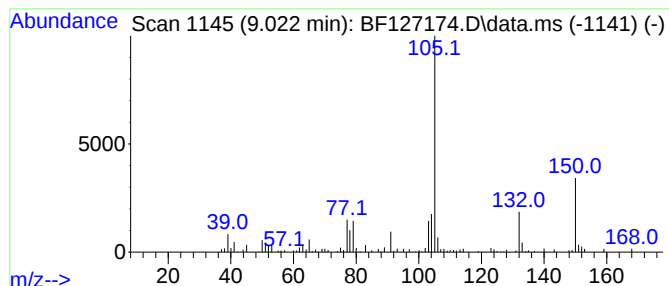
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 p-Tolylacetic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.022	6.38 ng	228559	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			p-Tolylacetic acid	150	C9H10O2	000622-47-9	64
2			Benzeneacetic acid, .alpha.-methyl-	150	C9H10O2	000492-37-5	62
3			para-Methylbenzyl formate	150	C9H10O2	1000368-93-7	58
4			o-Tolylacetic acid	150	C9H10O2	000644-36-0	52
5			m-Tolylacetic acid	150	C9H10O2	000621-36-3	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
Data File : BF127174.D
Acq On : 03 Mar 2022 16:39
Operator : CG\JU
Sample : N1689-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-40

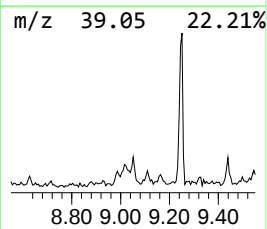
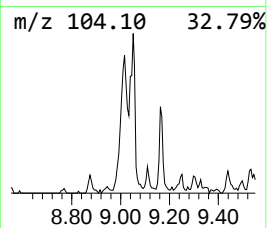
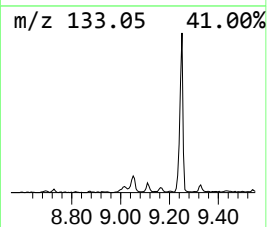
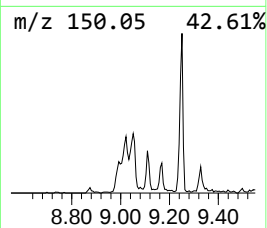
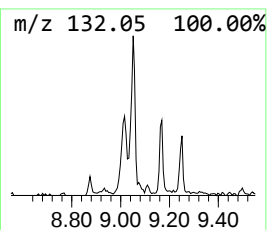
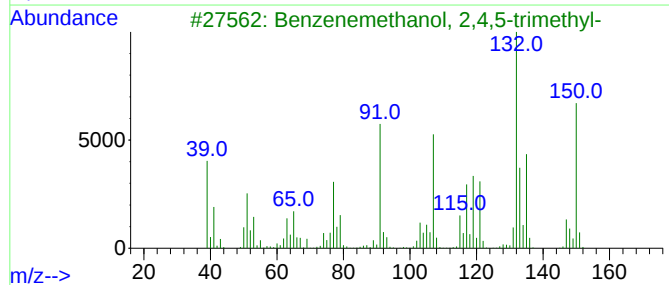
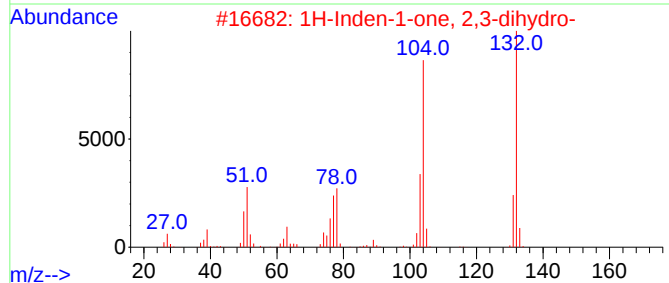
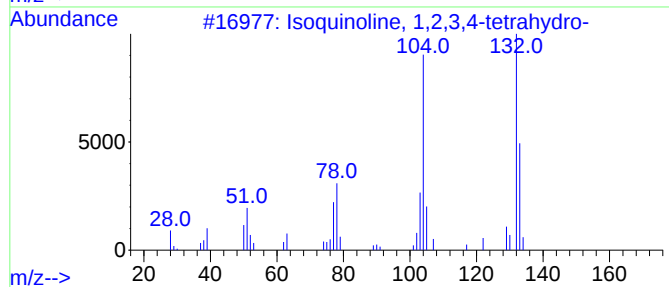
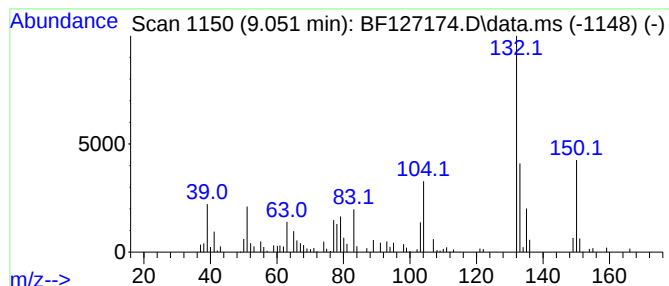
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Isoquinoline, 1,2,3,4-tetra... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.051	4.74 ng	181457	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isoquinoline, 1,2,3,4-tetrahydro-	133	C9H11N	000091-21-4	52
2			1H-Inden-1-one, 2,3-dihydro-	132	C9H8O	000083-33-0	38
3			Benzenemethanol, 2,4,5-trimethyl-	150	C10H14O	004393-05-9	38
4			Benzoic acid, 2,6-dimethyl-	150	C9H10O2	000632-46-2	38
5			1,3-Oxazolidine, 2,5-diphenyl-4-...	239	C16H17NO	1000138-86-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
Data File : BF127174.D
Acq On : 03 Mar 2022 16:39
Operator : CG\JU
Sample : N1689-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

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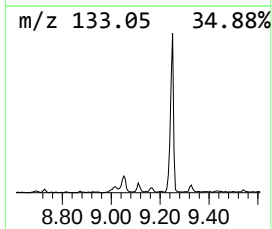
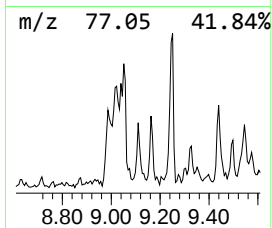
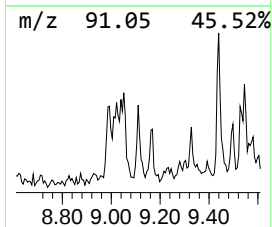
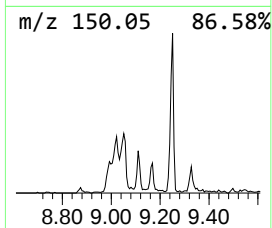
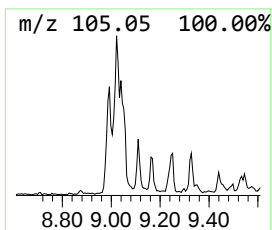
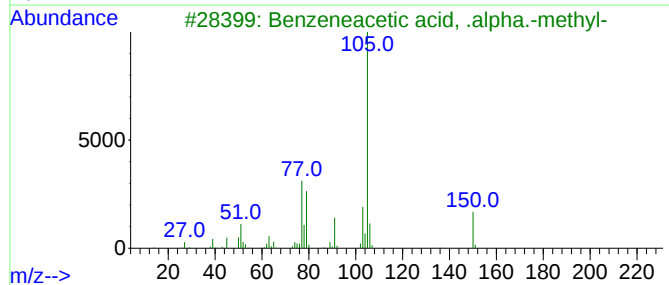
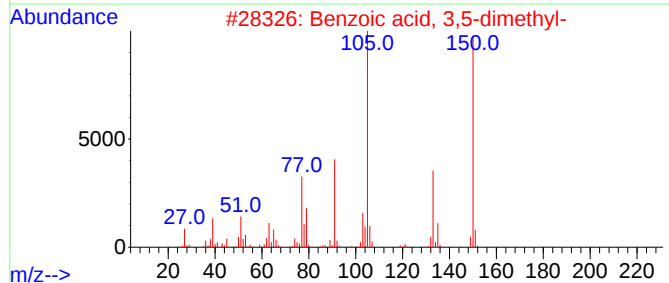
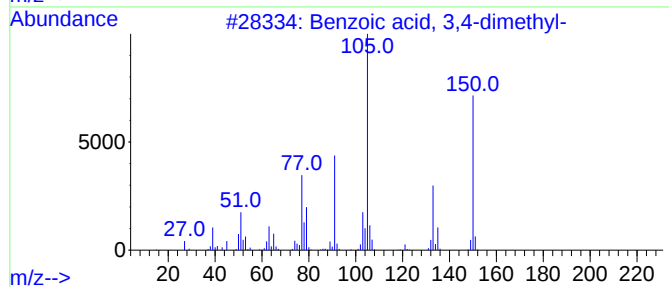
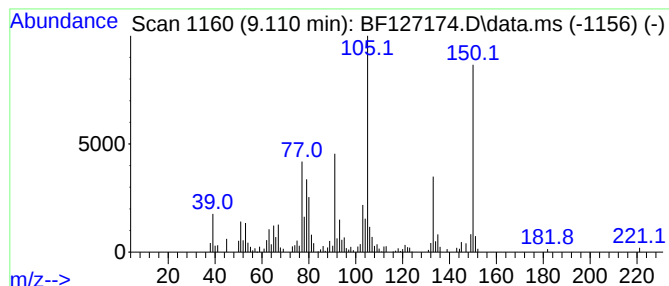
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Benzoic acid, 3,4-dimethyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.110	2.77 ng	106181	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 3,4-dimethyl-	150	C9H10O2	000619-04-5	93
2			Benzoic acid, 3,5-dimethyl-	150	C9H10O2	000499-06-9	93
3			Benzeneacetic acid, .alpha.-methyl-	150	C9H10O2	000492-37-5	81
4			Benzoic acid, 2,5-dimethyl-	150	C9H10O2	000610-72-0	74
5			p-Tolylacetic acid	150	C9H10O2	000622-47-9	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
Data File : BF127174.D
Acq On : 03 Mar 2022 16:39
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Sample : N1689-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

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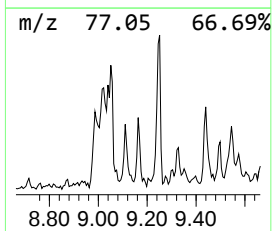
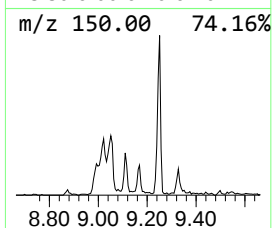
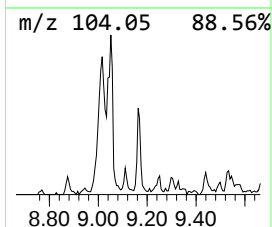
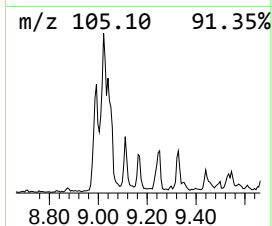
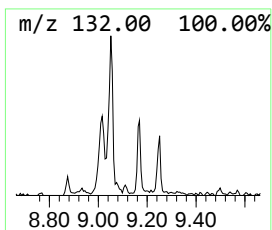
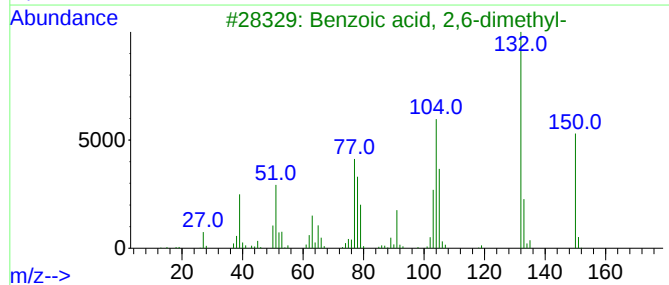
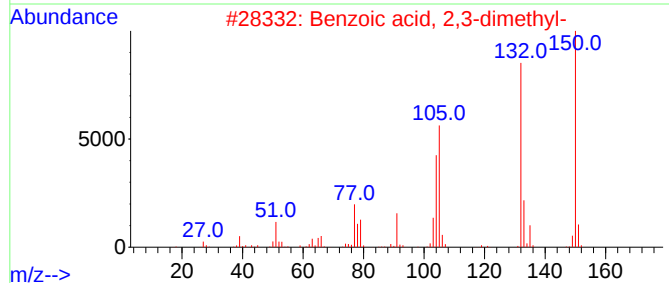
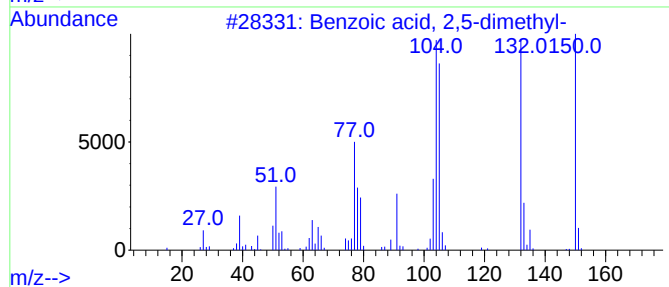
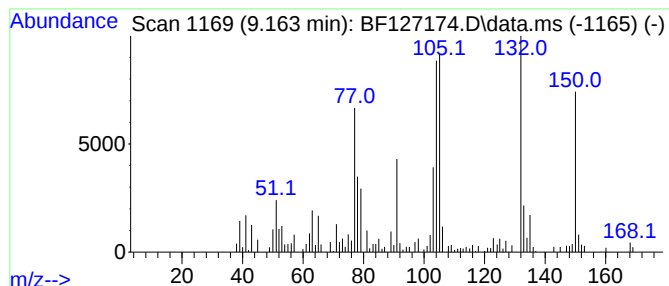
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Benzoic acid, 2,5-dimethyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.163	2.31 ng	88472	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2,5-dimethyl-	150	C9H10O2	000610-72-0	95
2			Benzoic acid, 2,3-dimethyl-	150	C9H10O2	000603-79-2	93
3			Benzoic acid, 2,6-dimethyl-	150	C9H10O2	000632-46-2	87
4			Benzoic acid, 2,4-dimethyl-	150	C9H10O2	000611-01-8	87
5			Formic acid, 1-phenylethyl ester	150	C9H10O2	1000368-94-1	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
Data File : BF127174.D
Acq On : 03 Mar 2022 16:39
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Misc :
ALS Vial : 5 Sample Multiplier: 1

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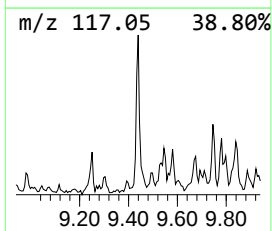
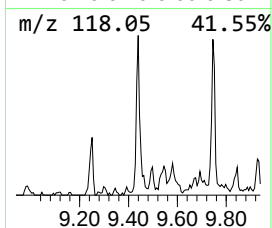
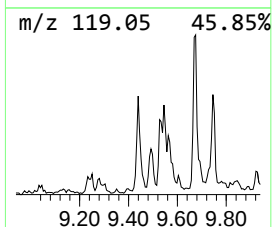
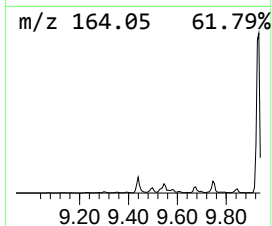
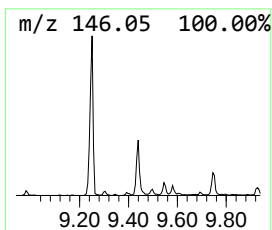
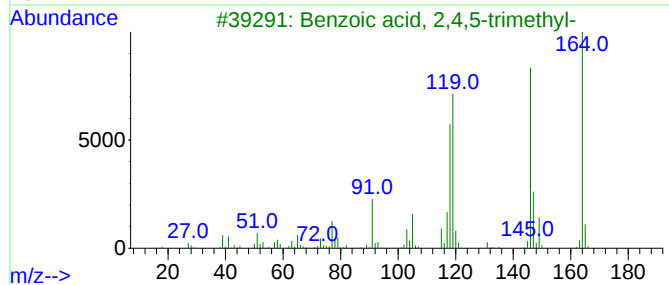
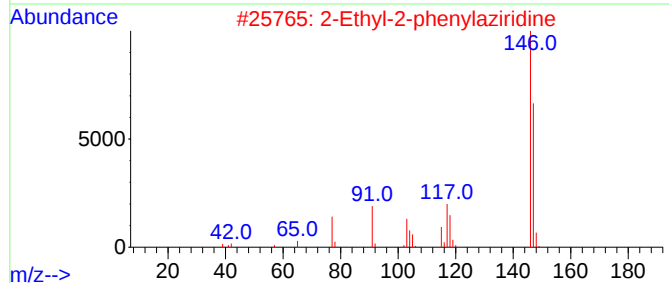
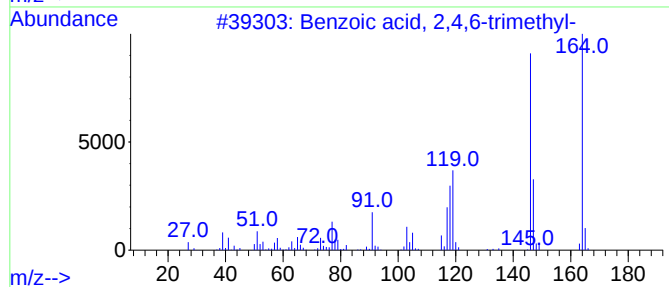
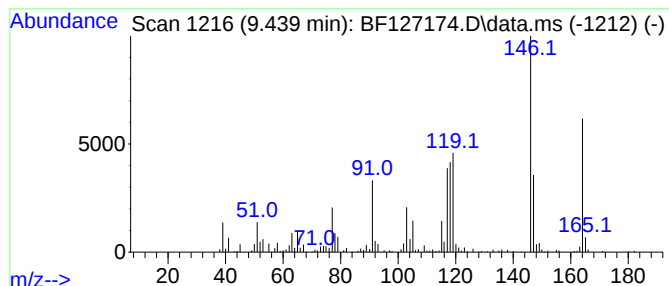
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Benzoic acid, 2,4,6-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.439	5.01 ng	191899	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2,4,6-trimethyl-	164	C10H12O2	000480-63-7	90
2			2-Ethyl-2-phenylaziridine	147	C10H13N	000768-82-1	45
3			Benzoic acid, 2,4,5-trimethyl-	164	C10H12O2	000528-90-5	43
4			6-Hydroxy-2-methylindole	147	C9H9NO	054584-22-4	38
5			1H-Indole, 2,3-dihydro-5-nitro-	164	C8H8N2O2	032692-19-6	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
Data File : BF127174.D
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Operator : CG\JU
Sample : N1689-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

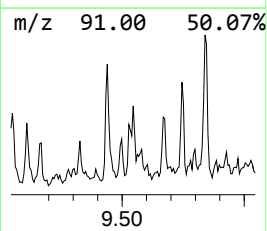
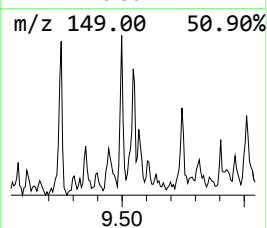
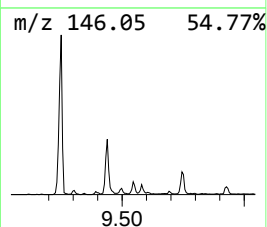
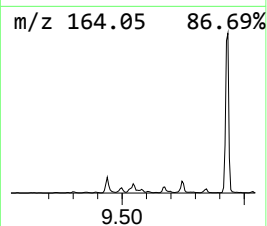
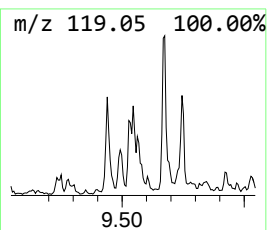
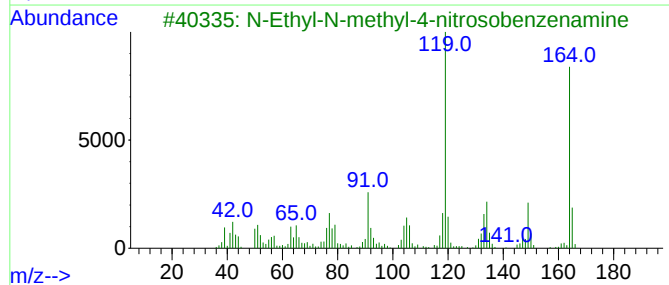
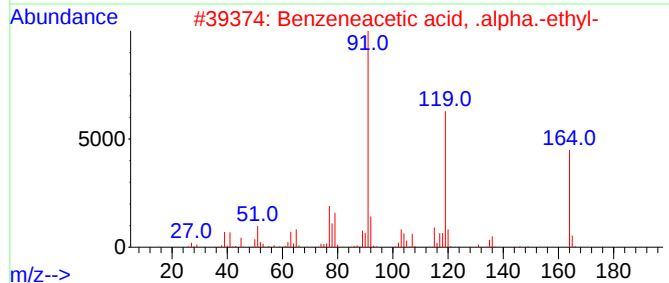
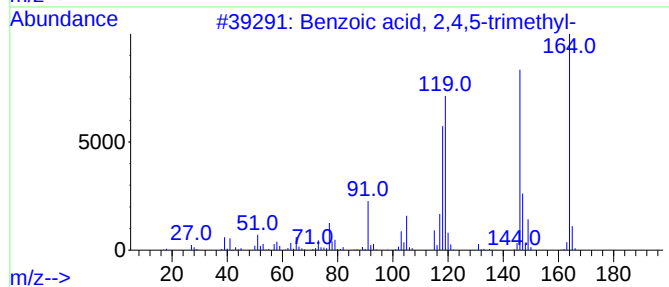
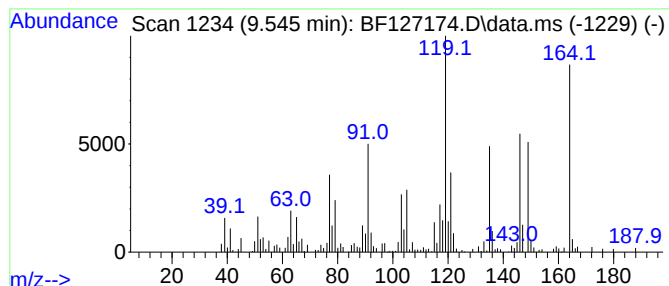
Instrument :
BNA_F
ClientSampleId :
MW-40

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Benzoic acid, 2,4,5-trimethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.545	3.53 ng	135187	Acenaphthene-d10	9.933	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2,4,5-trimethyl-	164	C10H12O2	000528-90-5	58
2	Benzeneacetic acid, .alpha.-ethyl-	164	C10H12O2	000090-27-7	55
3	N-Ethyl-N-methyl-4-nitrosobenzen...	164	C9H12N2O	036479-98-8	46
4	Benzamide, 4-methyl-	135	C8H9NO	000619-55-6	38
5	3-Allyl-6-methoxyphenol	164	C10H12O2	000501-19-9	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
Data File : BF127174.D
Acq On : 03 Mar 2022 16:39
Operator : CG\JU
Sample : N1689-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-40

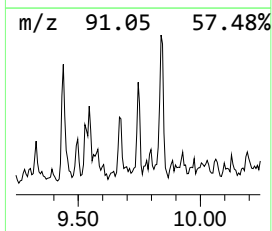
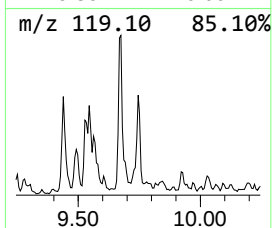
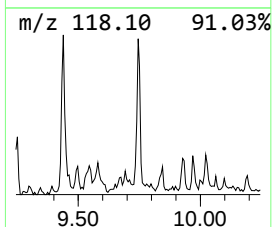
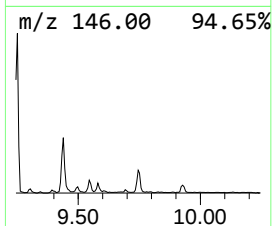
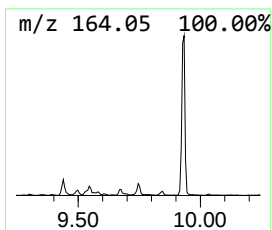
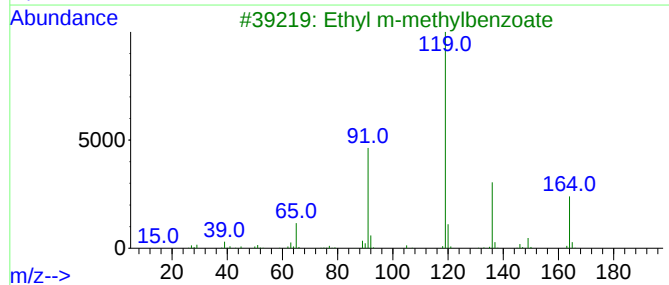
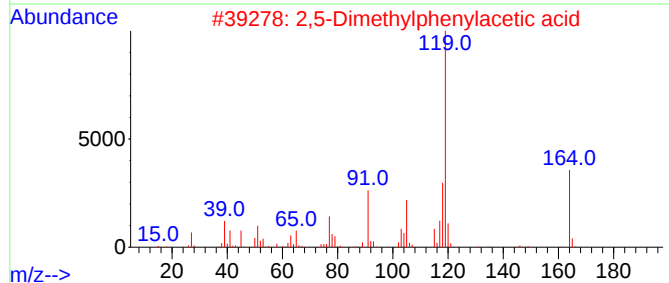
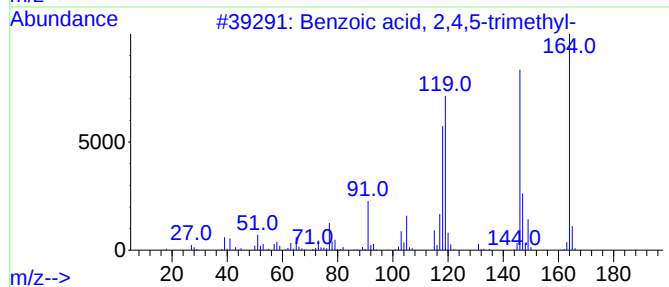
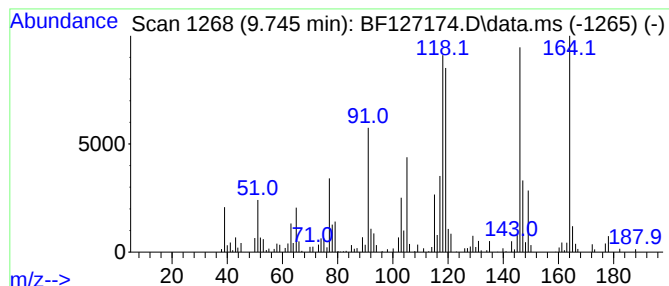
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 2,5-Dimethylphenylacetic acid Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.745	3.35 ng	128117	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2,4,5-trimethyl-	164	C10H12O2	000528-90-5	90
2			2,5-Dimethylphenylacetic acid	164	C10H12O2	1000342-65-5	50
3			Ethyl m-methylbenzoate	164	C10H12O2	000120-33-2	41
4			Ethyl 4-methylbenzoate	164	C10H12O2	000094-08-6	38
5			Phenol, 2-methoxy-4-(1-propenyl)-	164	C10H12O2	000097-54-1	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
Data File : BF127174.D
Acq On : 03 Mar 2022 16:39
Operator : CG\JU
Sample : N1689-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-40

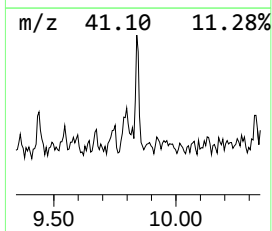
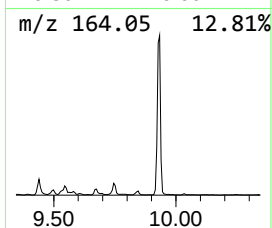
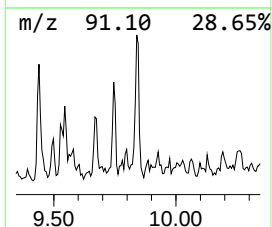
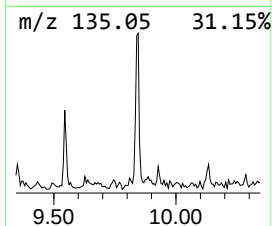
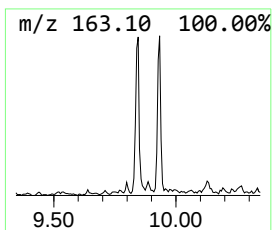
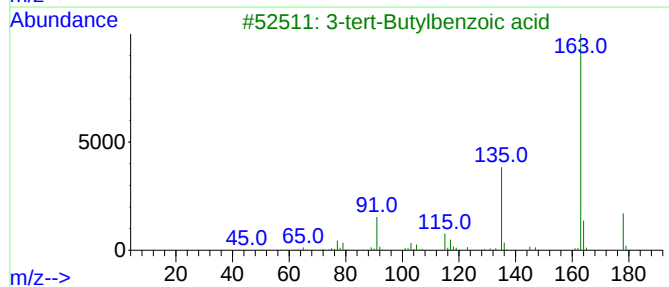
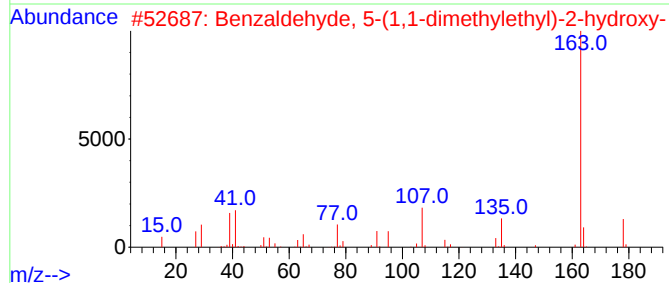
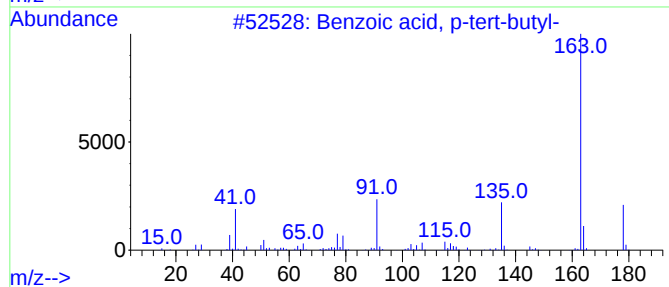
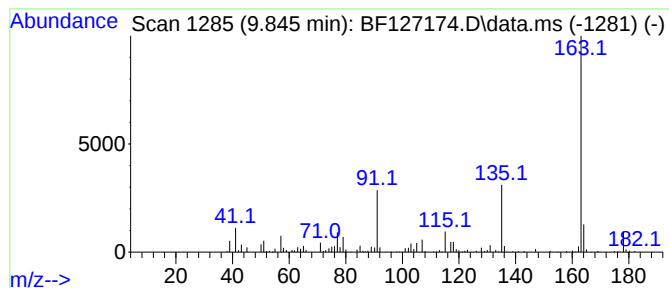
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Benzoic acid, p-tert-butyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.845	4.34 ng	166094	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	90
2			Benzaldehyde, 5-(1,1-dimethyleth...	178	C11H14O2	002725-53-3	59
3			3-tert-Butylbenzoic acid	178	C11H14O2	007498-54-6	53
4			2-tert-Butyl-4-ethylphenol, 0-is...	264	C16H24O3	1000487-42-5	53
5			3-pyridinecarbonitrile, 2-amino-...	163	C8H9N3O	1010404-44-3	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
 Data File : BF127174.D
 Acq On : 03 Mar 2022 16:39
 Operator : CG\JU
 Sample : N1689-04
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-40

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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
2-Butanol, 2,3-...	3.240	10.7	ng	274715	1	6.886	515875	20.0
Propane, 2-meth...	4.416	5.5	ng	141039	1	6.886	515875	20.0
unknown4.504	4.504	7.6	ng	197135	1	6.886	515875	20.0
unknown6.710	6.710	5.6	ng	144709	1	6.886	515875	20.0
unknown6.945	6.945	2.7	ng	69413	1	6.886	515875	20.0
2-Cyclopenten-1...	7.034	4.0	ng	104060	1	6.886	515875	20.0
unknown7.086	7.086	12.0	ng	310335	1	6.886	515875	20.0
Hexanoic acid, ...	7.157	16.5	ng	425288	1	6.886	515875	20.0
unknown7.528	7.528	23.2	ng	832205	2	8.169	716935	20.0
unknown7.739	7.739	6.6	ng	237761	2	8.169	716935	20.0
unknown8.098	8.098	2.6	ng	92572	2	8.169	716935	20.0
m-Tolylacetic acid	8.986	3.4	ng	122864	2	8.169	716935	20.0
p-Tolylacetic acid	9.022	6.4	ng	228559	2	8.169	716935	20.0
Isoquinoline, 1...	9.051	4.7	ng	181457	3	9.933	765933	20.0
Benzoic acid, 3...	9.110	2.8	ng	106181	3	9.933	765933	20.0
Benzoic acid, 2...	9.163	2.3	ng	88472	3	9.933	765933	20.0
Benzoic acid, 2...	9.439	5.0	ng	191899	3	9.933	765933	20.0
Benzoic acid, 2...	9.545	3.5	ng	135187	3	9.933	765933	20.0
2,5-Dimethylphe...	9.745	3.4	ng	128117	3	9.933	765933	20.0
Benzoic acid, p...	9.845	4.3	ng	166094	3	9.933	765933	20.0