

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016608.D
 Acq On : 30 Sep 2021 20:22
 Operator : CG/JU
 Sample : M3962-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 UNDERPASS

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 1 % 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_N\METHODS\8270-SIM-BN100121.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BN016608.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.816	77	80	87	rBV	7686	26747	7.55%	0.898%
2	3.908	87	90	105	rVB	25335	89064	25.14%	2.989%
3	4.821	185	189	197	rBV	36276	85790	24.22%	2.880%
4	5.005	206	209	212	rBV	2759	6757	1.91%	0.227%
5	5.272	234	238	244	rBV	7160	17797	5.02%	0.597%
6	5.365	245	248	256	rVB	3212	8849	2.50%	0.297%
7	6.831	403	407	417	rVB2	5879	19497	5.50%	0.654%
8	6.978	420	423	435	rBV2	3974	12243	3.46%	0.411%
9	7.264	451	454	460	rVB	6718	14526	4.10%	0.488%
10	7.642	490	495	500	rBV	47346	95637	27.00%	3.210%
11	8.455	574	579	582	rBV2	2894	7800	2.20%	0.262%
12	8.784	602	605	609	rBV	21905	39821	11.24%	1.337%
13	9.443	654	657	661	rVB	4502	8649	2.44%	0.290%
14	10.191	713	716	719	rBV	7543	14836	4.19%	0.498%
15	10.406	730	733	736	rBV	99772	177105	50.00%	5.945%
16	10.457	736	737	740	rVB	11342	15956	4.50%	0.536%
17	12.007	918	932	942	rBV	45146	74531	21.04%	2.502%
18	12.898	1071	1075	1078	rVB	83963	146456	41.34%	4.916%
19	14.268	1180	1183	1186	rBV	130886	195131	55.08%	6.550%
20	14.332	1186	1188	1192	rVB3	4744	8304	2.34%	0.279%
21	14.560	1204	1206	1210	rVB3	4552	8407	2.37%	0.282%
22	14.954	1235	1237	1239	rVB	5399	7937	2.24%	0.266%
23	15.042	1239	1244	1247	rBV3	3057	9777	2.76%	0.328%
24	15.233	1256	1259	1260	rBV2	4137	7859	2.22%	0.264%
25	15.322	1264	1266	1268	rVB	8094	12283	3.47%	0.412%
26	15.626	1288	1290	1295	rVB3	6598	15235	4.30%	0.511%
27	15.766	1298	1301	1305	rVB3	16662	30821	8.70%	1.035%
28	15.867	1305	1309	1312	rBV3	3046	8126	2.29%	0.273%
29	15.956	1313	1316	1319	rBV	24693	42288	11.94%	1.419%
30	16.324	1340	1346	1348	rBV3	5372	16991	4.80%	0.570%
31	16.384	1348	1351	1356	rVB3	7670	18412	5.20%	0.618%
32	16.847	1386	1389	1393	rVB	4374	9307	2.63%	0.312%
33	17.017	1400	1403	1406	rBV	95345	174614	49.29%	5.861%
34	17.066	1406	1407	1409	rVV	29229	30567	8.63%	1.026%
35	17.151	1412	1414	1417	rVB	19778	30911	8.73%	1.038%
36	17.224	1417	1420	1422	rBV	6111	10351	2.92%	0.347%

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37	17.431	1434	1437	1440	rBV2	8157	13158	3.71%	0.442%
38	17.954	1477	1480	1483	rBV	11207	18086	5.11%	0.607%
39	18.313	1541	1545	1550	rVB	3017	3874	1.09%	0.130%
40	18.412	1560	1565	1568	rBV2	2648	3761	1.06%	0.126%
41	18.834	1646	1650	1656	rBV2	2648	3844	1.09%	0.129%
42	19.068	1690	1697	1702	rBV	127914	183521	51.81%	6.160%
43	19.246	1728	1733	1745	rBV	10472	15214	4.29%	0.511%
44	19.460	1771	1776	1781	rBV	10715	13195	3.72%	0.443%
45	19.678	1814	1820	1833	rBV	123666	151291	42.71%	5.078%
46	20.006	1884	1886	1888	rBV	10973	14801	4.18%	0.497%
47	20.972	1975	1977	1980	rBV	8749	14431	4.07%	0.484%
48	21.025	1980	1982	1989	rVV	13391	22408	6.33%	0.752%
49	21.174	1993	1996	1998	rVV	30729	39592	11.18%	1.329%
50	21.238	1998	2002	2004	rVV2	134612	211414	59.68%	7.096%
51	21.312	2007	2009	2012	rVB	6154	8714	2.46%	0.292%
52	21.769	2049	2052	2058	rBV	243540	354242	100.00%	11.890%
53	21.992	2070	2073	2075	rVB	9622	14892	4.20%	0.500%
54	22.321	2101	2104	2109	rVB	10758	20453	5.77%	0.687%
55	22.810	2224	2230	2236	rBV	4125	6186	1.75%	0.208%
56	22.851	2238	2242	2253	rVB2	5290	7620	2.15%	0.256%
57	23.484	2415	2427	2453	rVB	110385	208507	58.86%	6.999%
58	24.285	2649	2661	2684	rVB	67998	135497	38.25%	4.548%
59	25.774	3079	3096	3097	rBV2	4244	8370	2.36%	0.281%
60	26.459	3283	3296	3323	rVB	2234	6850	1.93%	0.230%

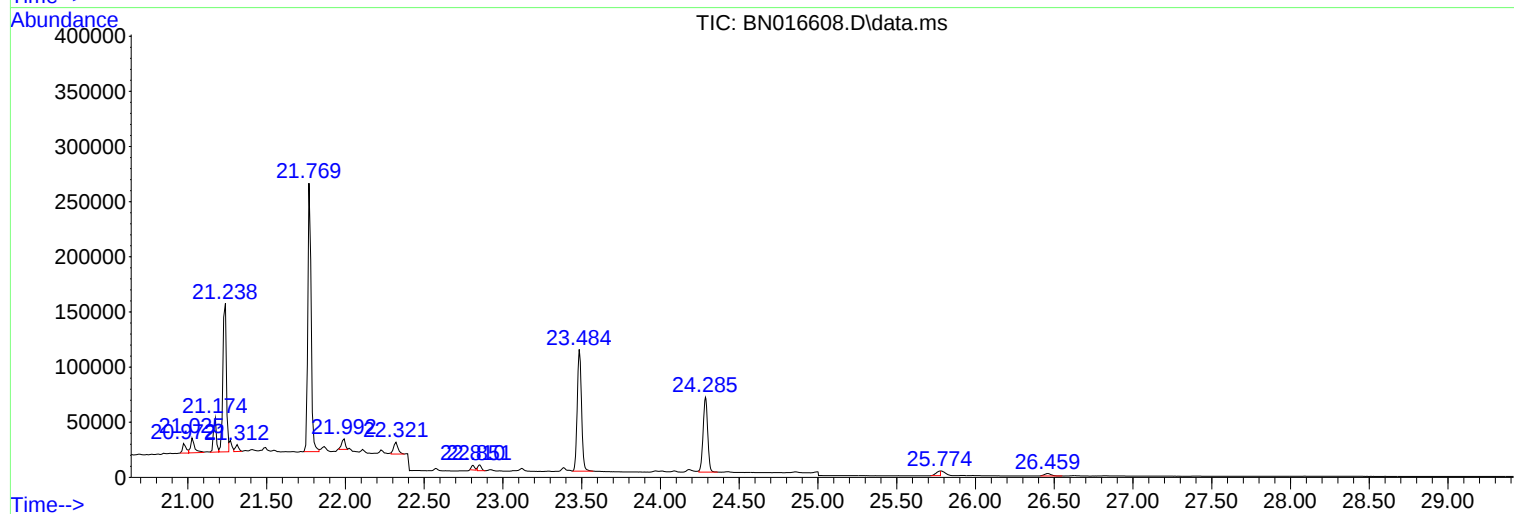
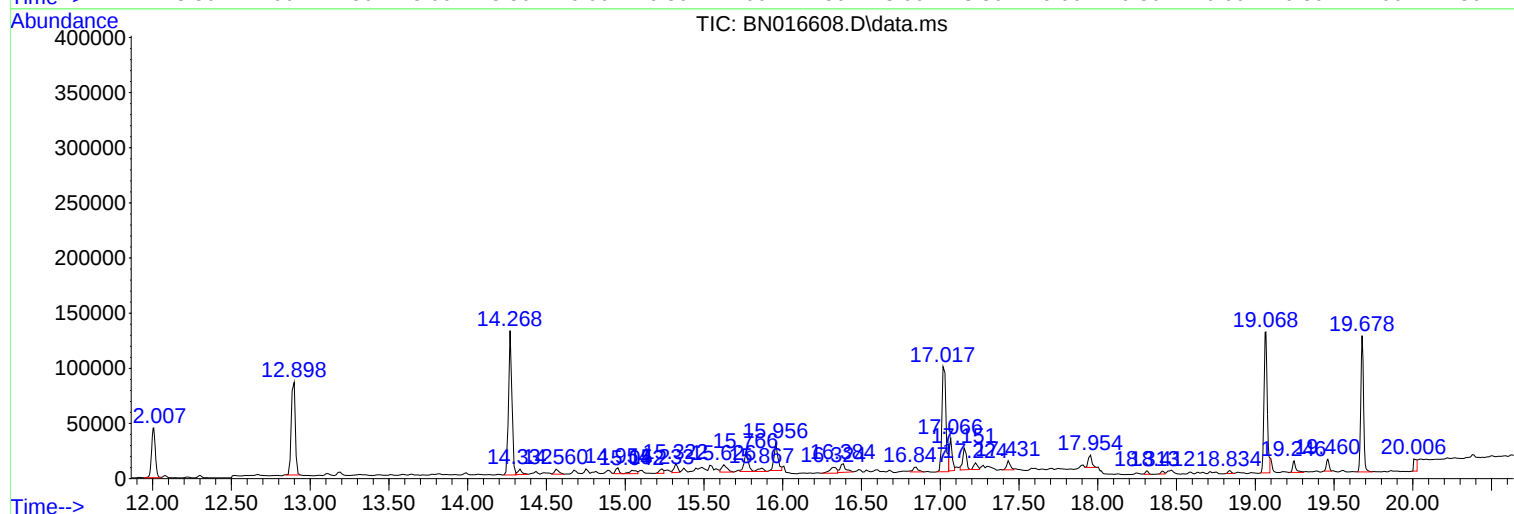
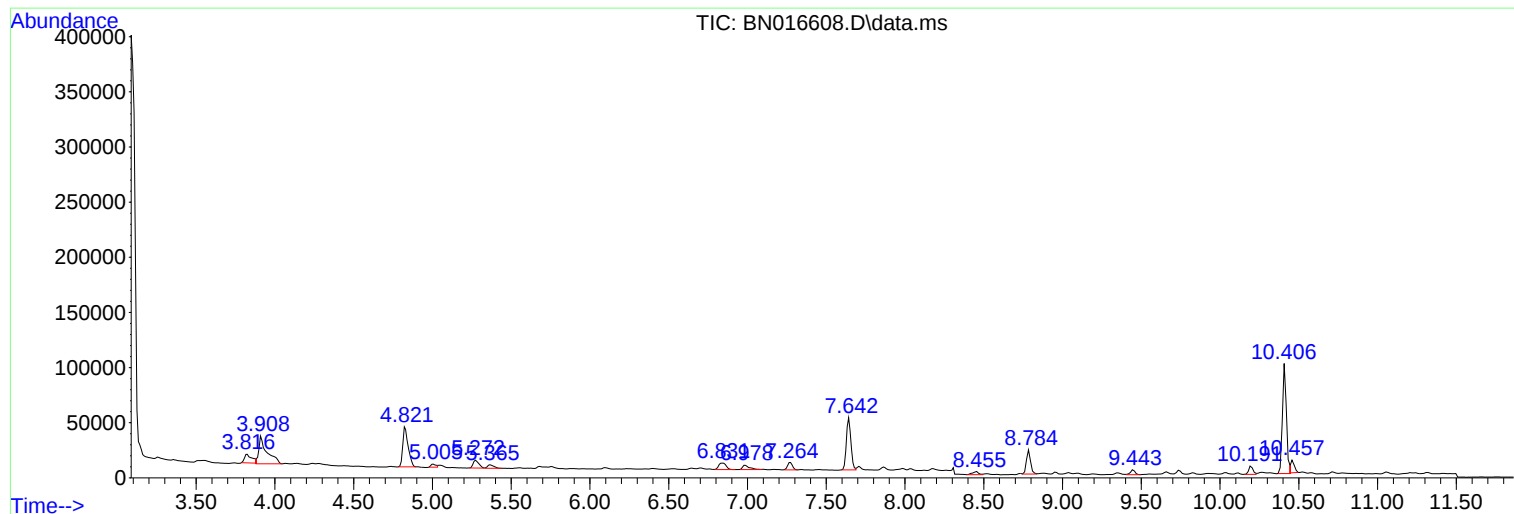
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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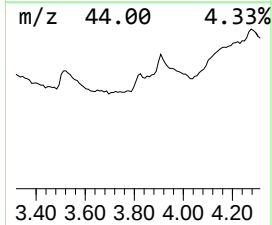
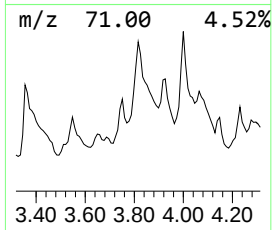
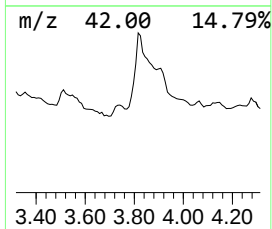
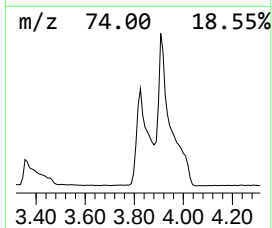
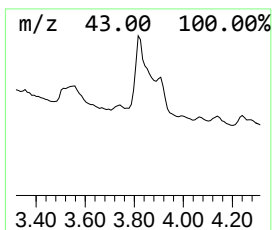
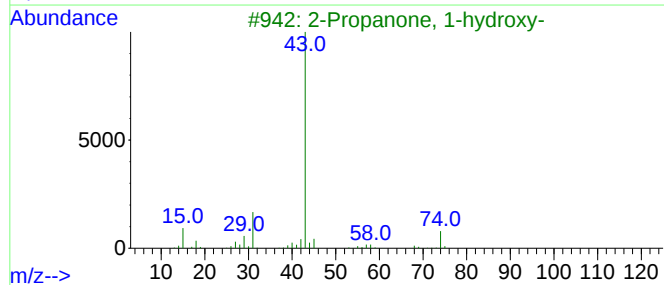
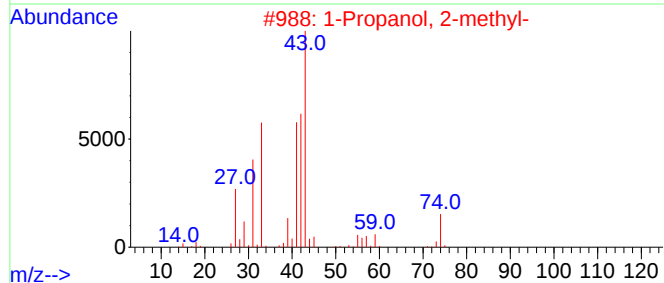
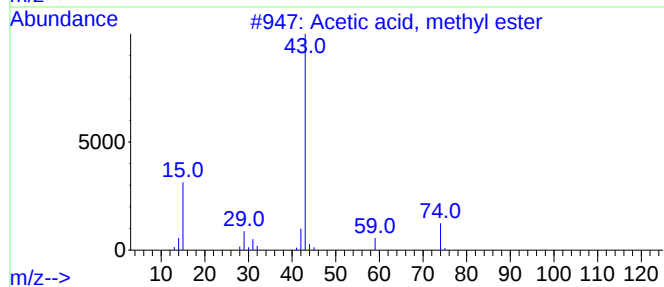
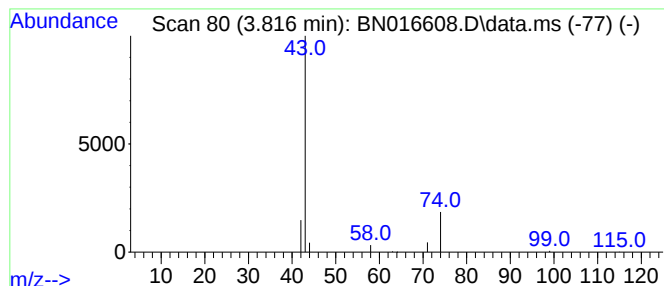
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Acetic acid, methyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.11 ng	26747	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, methyl ester	74	C3H6O2	000079-20-9	7
2			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	4
3			2-Propanone, 1-hydroxy-	74	C3H6O2	000116-09-6	4
4			Isobutane	58	C4H10	000075-28-5	4
5			Ethanone, 1-(3,3-dimethyloxiranyl)-	114	C6H10O2	004478-63-1	4



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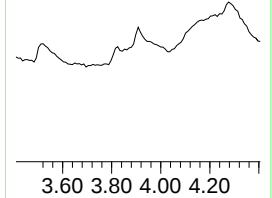
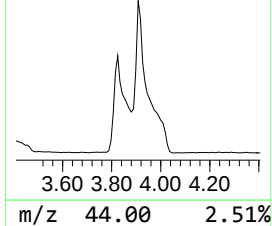
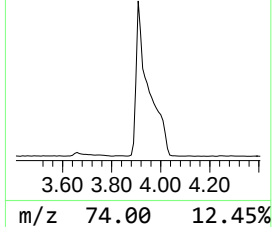
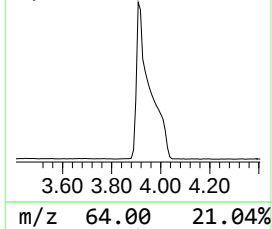
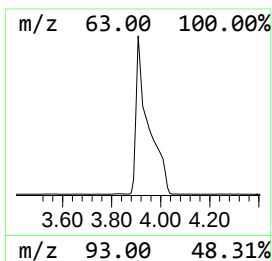
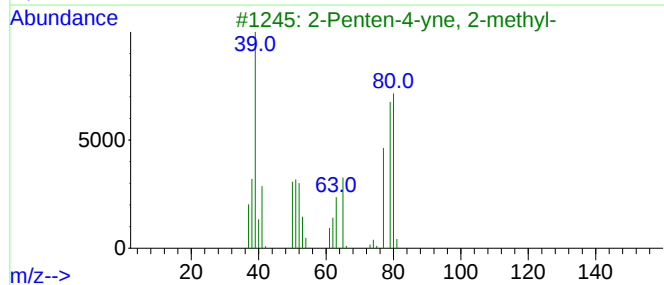
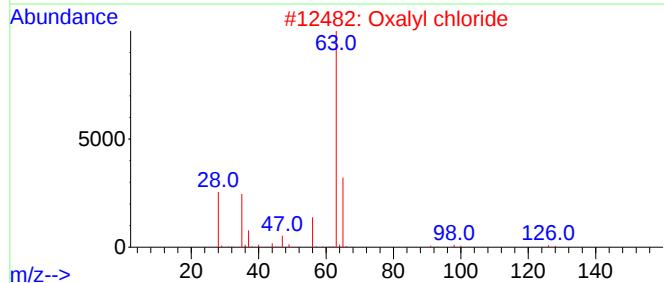
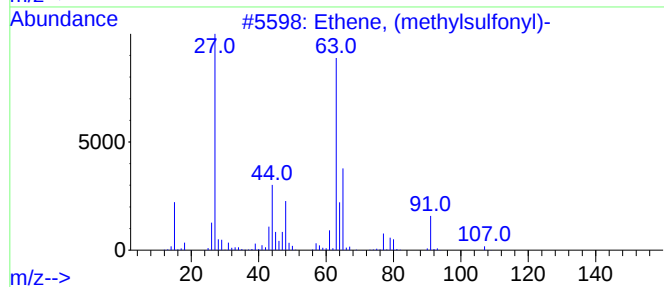
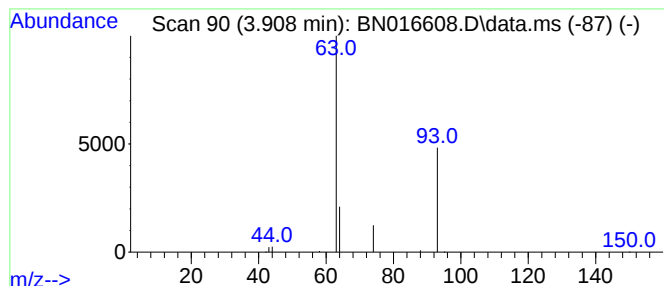
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethene, (methylsulfonyl)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.908	0.37 ng	89064	1,4-Dichlorobenzene-d4	7.642

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethene, (methylsulfonyl)-	106	C3H6O2S	003680-02-2	2
2		Oxalyl chloride	126	C2Cl2O2	000079-37-8	1
3		2-Penten-4-yne, 2-methyl-	80	C6H8	001595-53-5	1
4		Ethenesulfonyl chloride	126	C2H3ClO2S	006608-47-5	1
5		Chloro(prop-2-yn-1-yloxy)methanone	118	C4H3ClO2	035718-08-2	1



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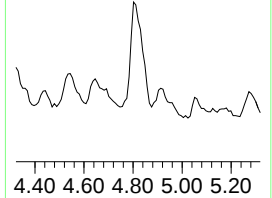
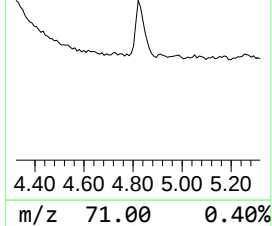
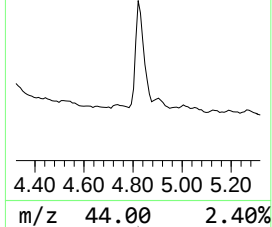
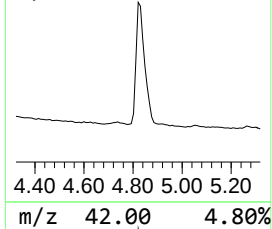
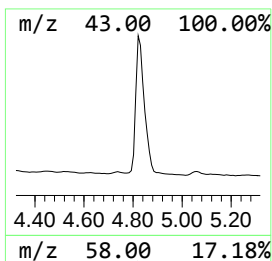
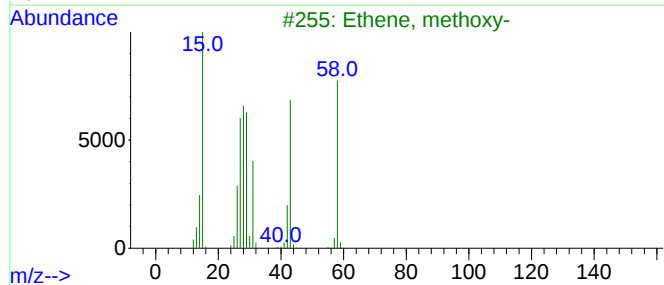
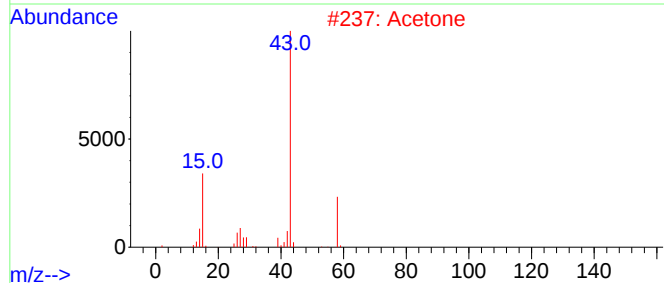
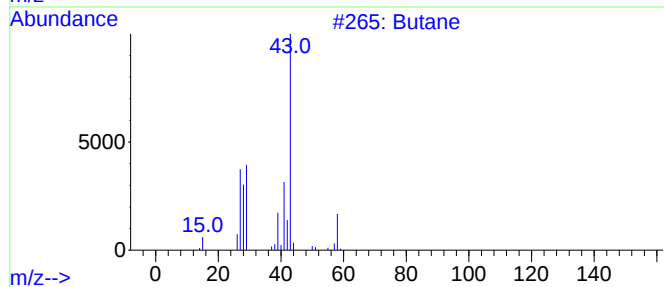
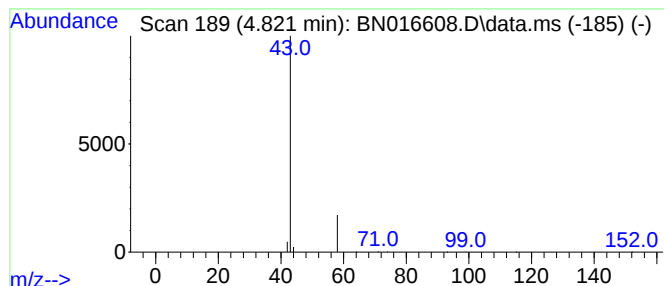
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.36 ng	85790	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	4
2			Acetone	58	C3H6O	000067-64-1	4
3			Ethene, methoxy-	58	C3H6O	000107-25-5	3
4			Diazene, dimethyl-	58	C2H6N2	000503-28-6	3
5			Hydrogen isocyanate	43	CHNO	000075-13-8	2



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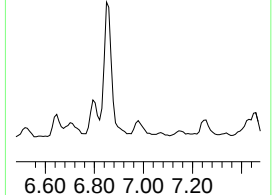
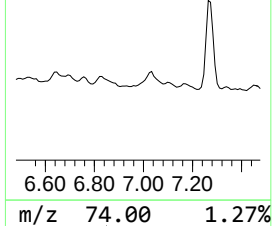
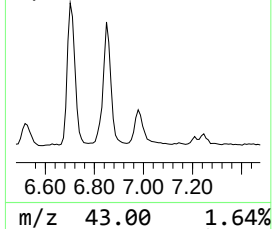
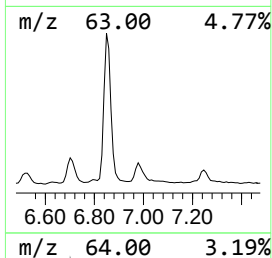
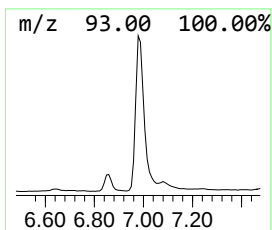
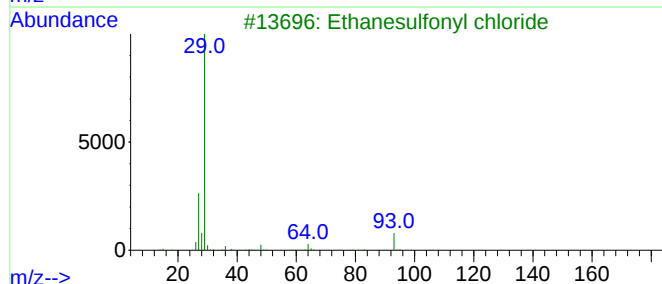
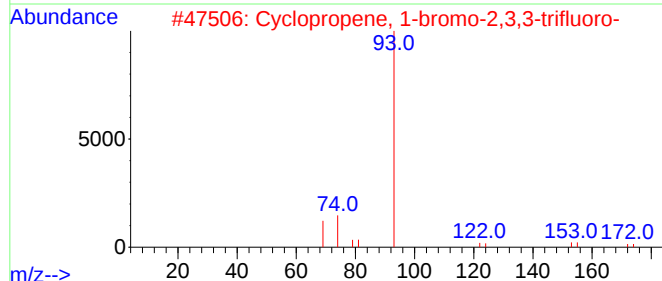
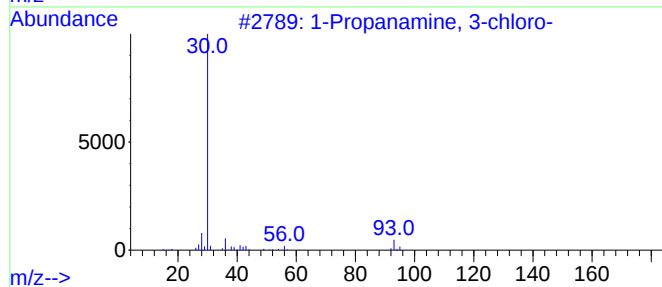
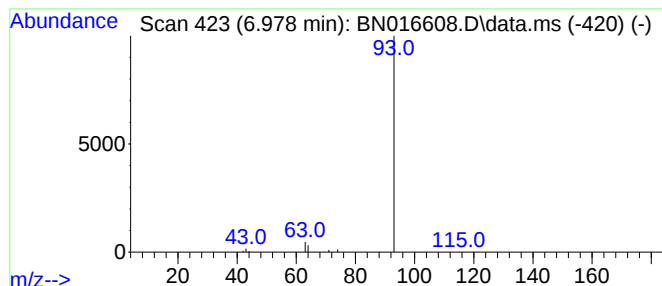
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Propanamine, 3-chloro- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.978	0.05 ng	12243	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propanamine, 3-chloro-	93	C3H8ClN	014753-26-5	1
2			Cyclopropene, 1-bromo-2,3,3-trif...	172	C3BrF3	029777-44-4	1
3			Ethanesulfonyl chloride	128	C2H5ClO2S	000594-44-5	1
4			Carbonochloridic acid, ethyl ester	108	C3H5ClO2	000541-41-3	1
5			Ethenesulfonyl chloride	126	C2H3ClO2S	006608-47-5	1



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UNDERPASS

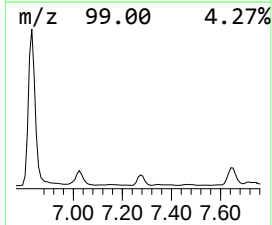
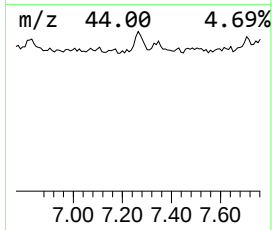
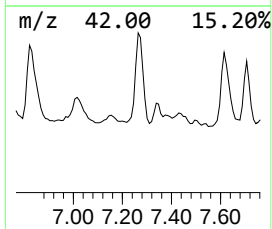
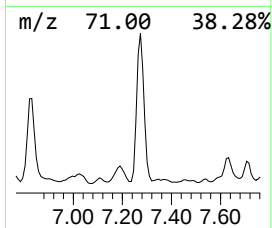
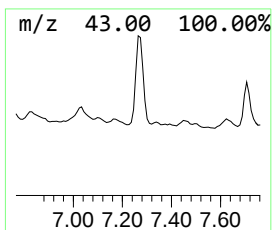
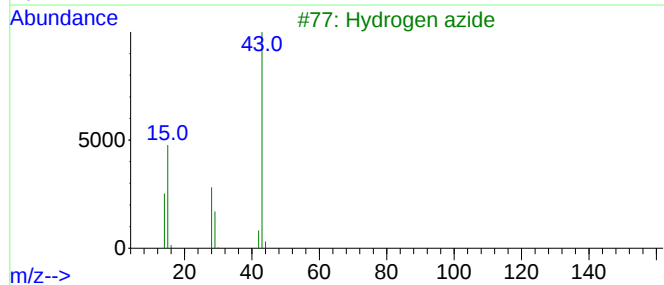
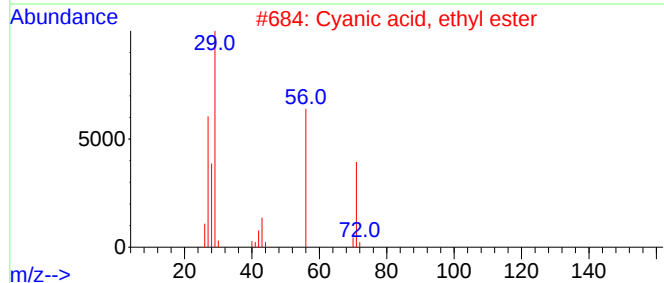
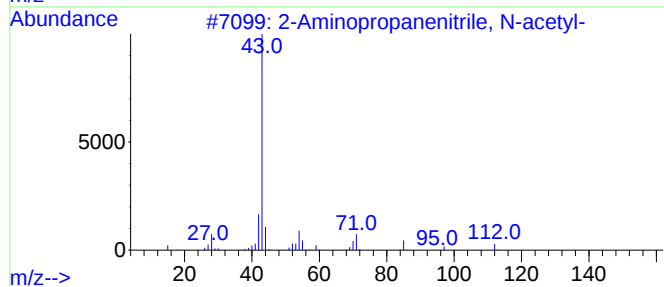
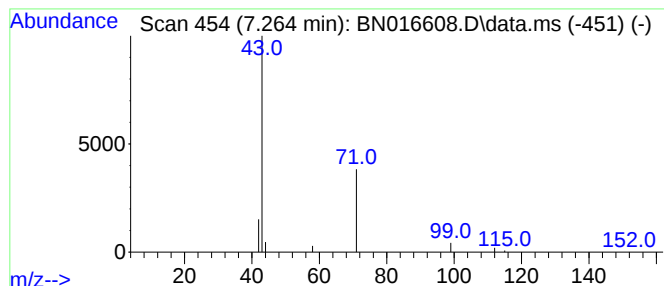
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 2-Aminopropanenitrile, N-ac... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.264	0.06 ng	14526	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Aminopropanenitrile, N-acetyl-	112	C5H8N2O	019861-71-3	4
2	Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	4
3	Hydrogen azide	43	HN3	007782-79-8	4
4	Isobutane	58	C4H10	000075-28-5	4
5	Decane, 2-methyl-	156	C11H24	006975-98-0	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016608.D
Acq On : 30 Sep 2021 20:22
Operator : CG/JU
Sample : M3962-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
UNDERPASS

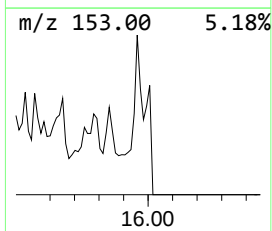
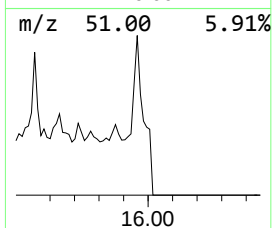
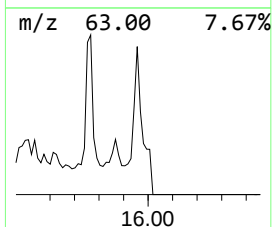
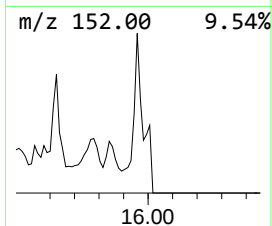
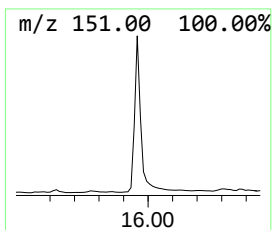
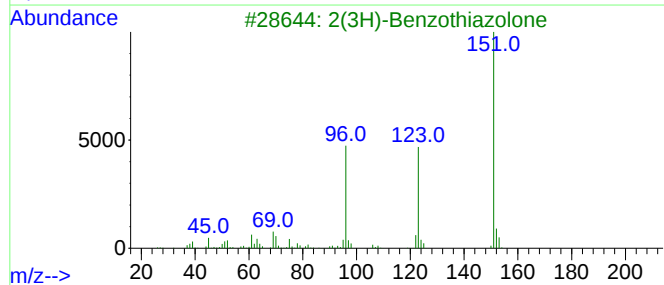
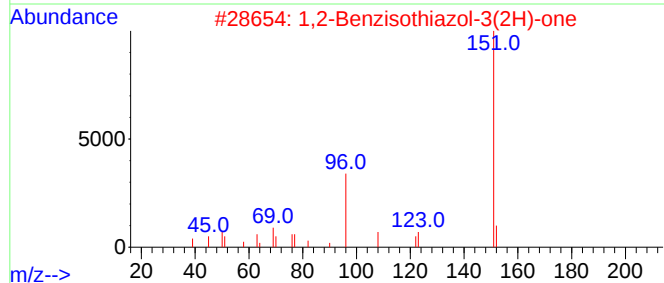
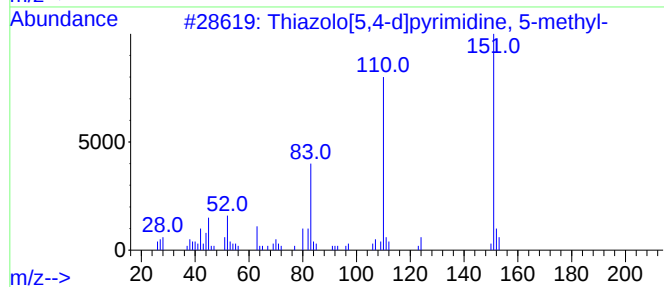
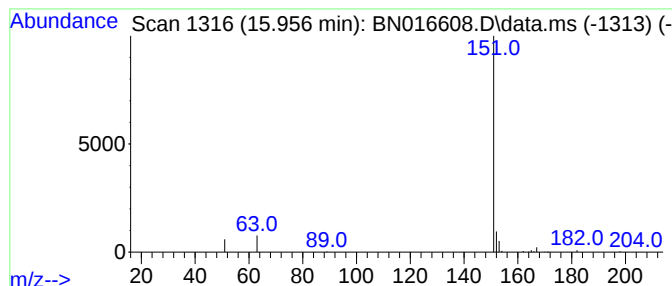
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Thiazolo[5,4-d]pyrimidine, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.956	0.10 ng	42288	Phenanthrene-d10	17.029

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiazolo[5,4-d]pyrimidine, 5-met...	151	C6H5N3S	013554-89-7	9
2			1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	9
3			2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	7
4			4-Mercaptoimidazo[4,5-c]pyridine	151	C6H5N3S	034550-51-1	7
5			2-Mercapto-1,3-benzoxazole	151	C7H5NOS	002382-96-9	7



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016608.D
Acq On : 30 Sep 2021 20:22
Operator : CG/JU
Sample : M3962-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

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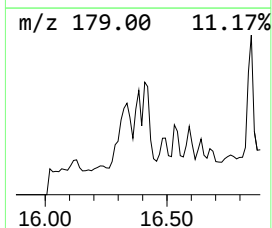
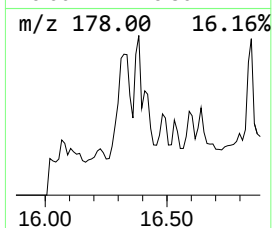
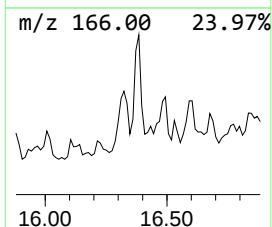
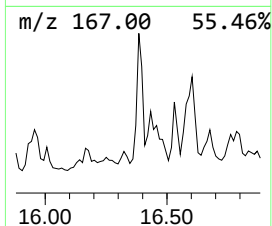
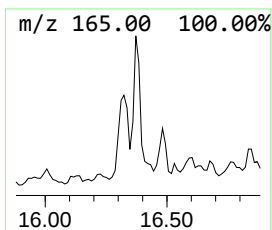
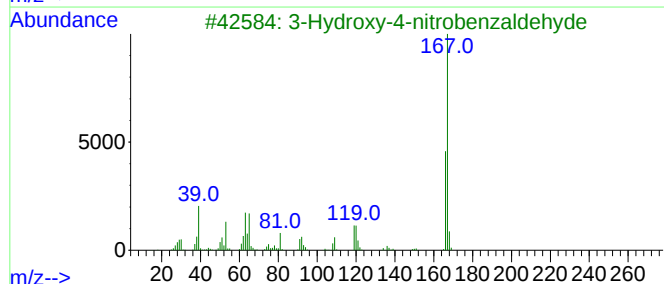
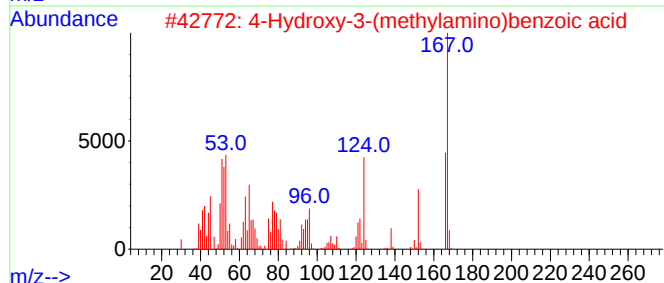
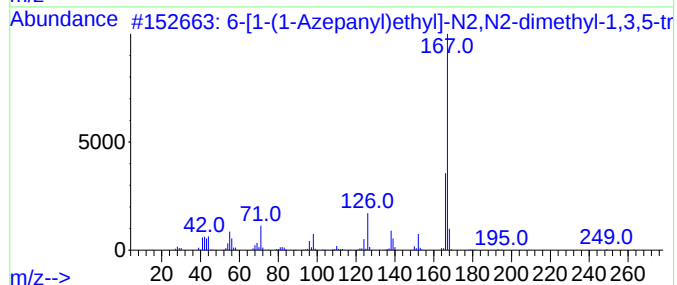
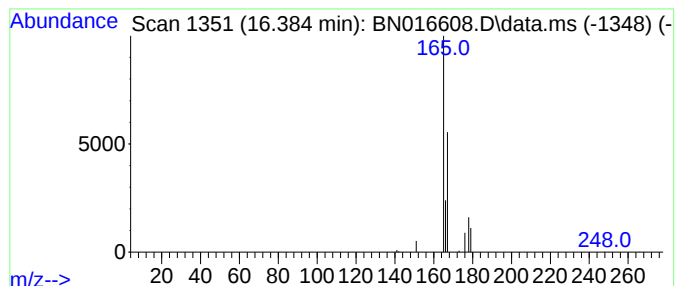
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 6-[1-(1-Azepanyl)ethyl]-N2,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.384	0.04 ng	18412	Phenanthrene-d10	17.029

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-[1-(1-Azepanyl)ethyl]-N2,N2-di...	264	C13H24N6	923208-22-4	7		
2	4-Hydroxy-3-(methylamino)benzoic...	167	C8H9NO3	000617-13-0	5		
3	3-Hydroxy-4-nitrobenzaldehyde	167	C7H5NO4	000704-13-2	5		
4	thiazole, 2-chloro-5-(methylthio)-	165	C4H4ClNS2	1000404-50-5	5		
5	2,3-Dichloromaleimide	165	C4HCl2NO2	001193-54-0	5		



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Operator : CG/JU
Sample : M3962-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

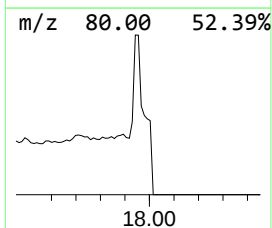
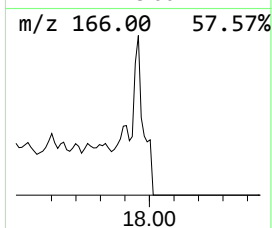
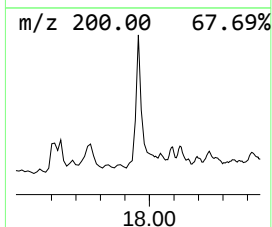
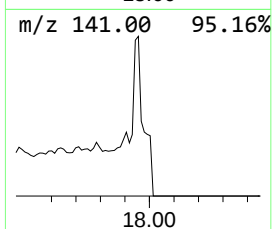
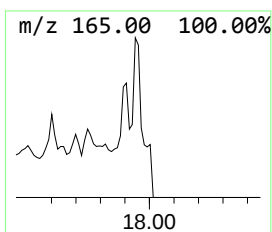
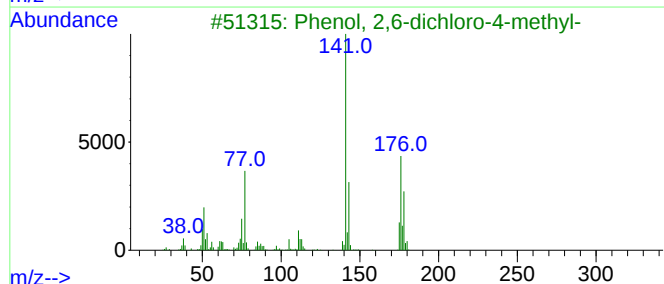
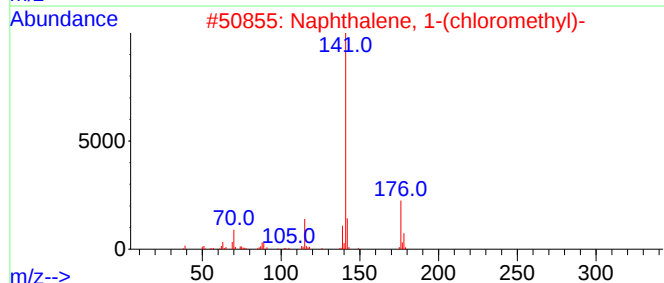
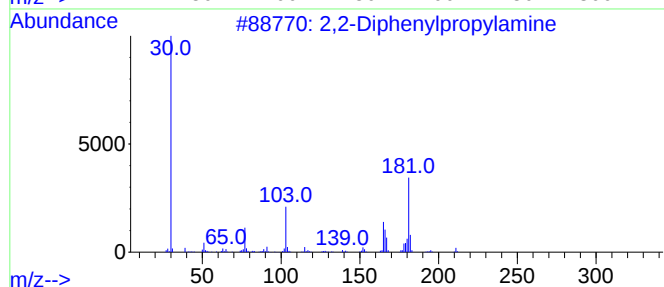
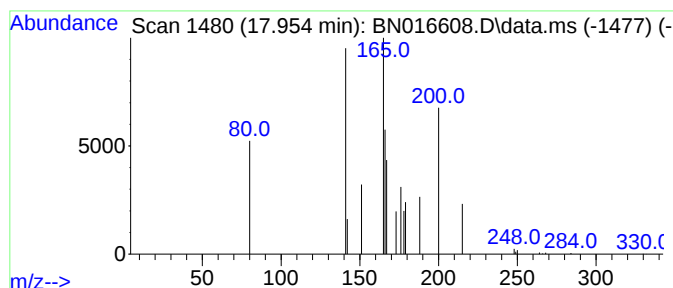
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2,2-Diphenylpropylamine Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.954	0.04 ng	18086	Phenanthrene-d10		17.029	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,2-Diphenylpropylamine		211	C15H17N	034611-07-9	23
2	Naphthalene, 1-(chloromethyl)-		176	C11H9Cl	000086-52-2	9
3	Phenol, 2,6-dichloro-4-methyl-		176	C7H6Cl2O	002432-12-4	9
4	4-Chlorophenoxyacetic acid, meth...		200	C9H9ClO3	1000362-94-5	9
5	Benzenesulfonyl chloride		176	C6H5ClO2S	000098-09-9	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Operator : CG/JU
Sample : M3962-01
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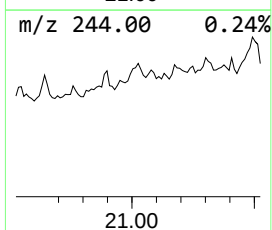
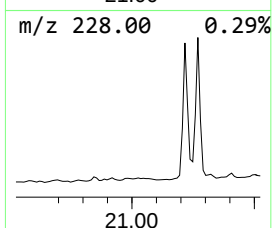
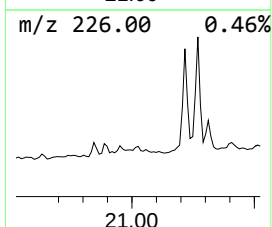
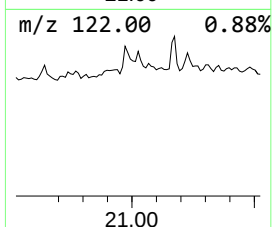
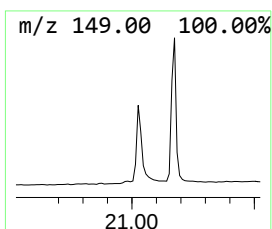
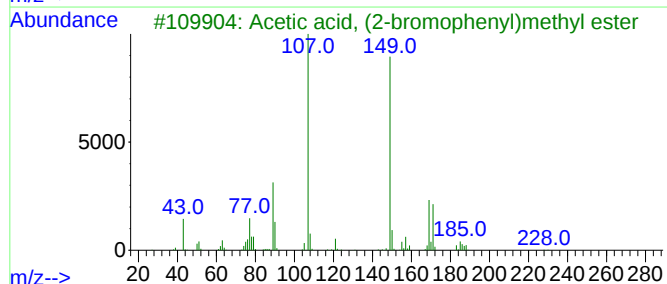
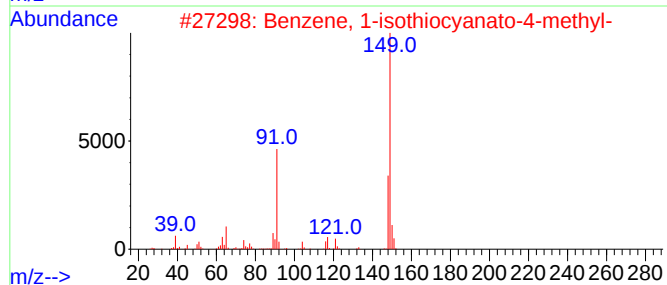
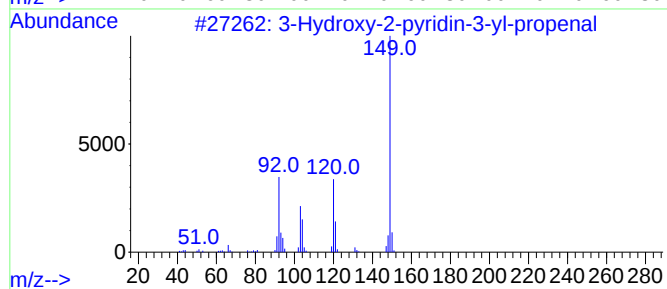
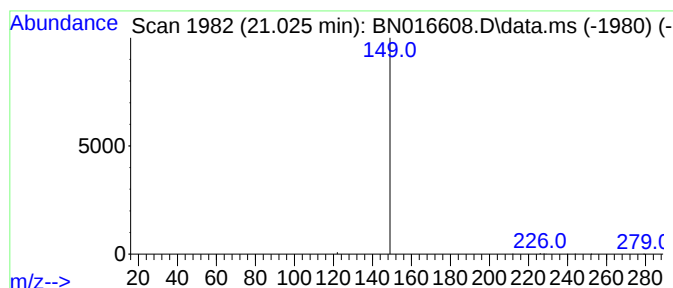
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 3-Hydroxy-2-pyridin-3-yl-pr... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.025	0.04 ng	22408	Chrysene-d12	21.238	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hydroxy-2-pyridin-3-yl-propenal	149	C8H7NO2	1000311-61-6	4
2	Benzene, 1-isothiocyanato-4-methyl-	149	C8H7NS	000622-59-3	4
3	Acetic acid, (2-bromophenyl)meth...	228	C9H9BrO2	1000368-71-4	3
4	(1R,4aR,7R,8aR)-7-(2-Hydroxyprop...	240	C15H28O2	004666-84-6	3
5	m-Tolyl isothiocyanate	149	C8H7NS	000621-30-7	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Misc :
ALS Vial : 13 Sample Multiplier: 1

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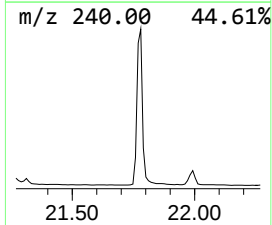
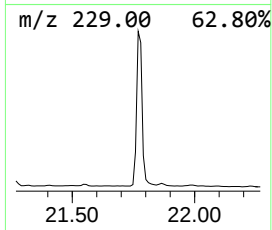
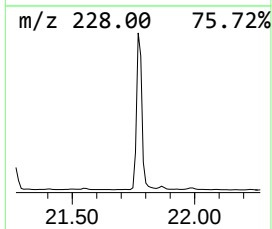
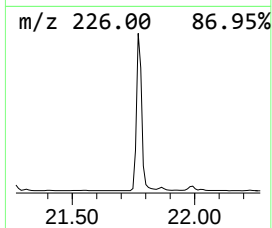
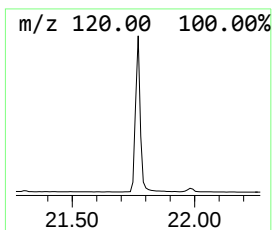
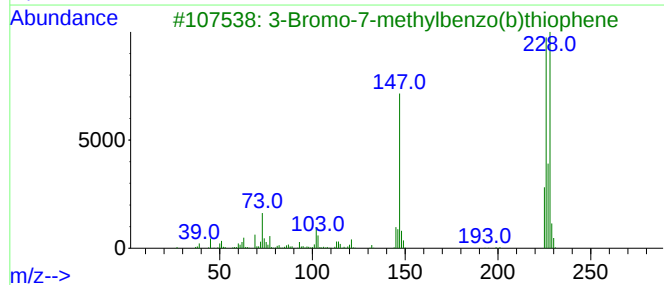
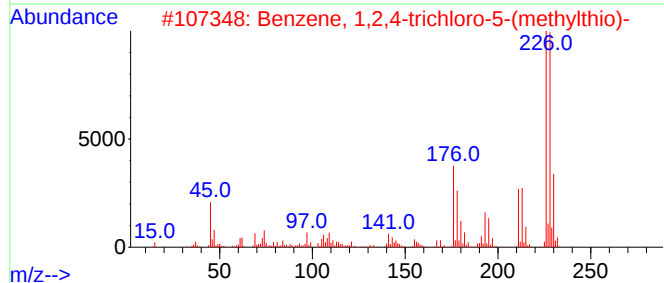
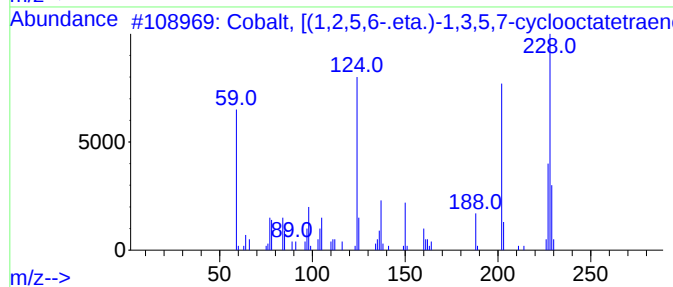
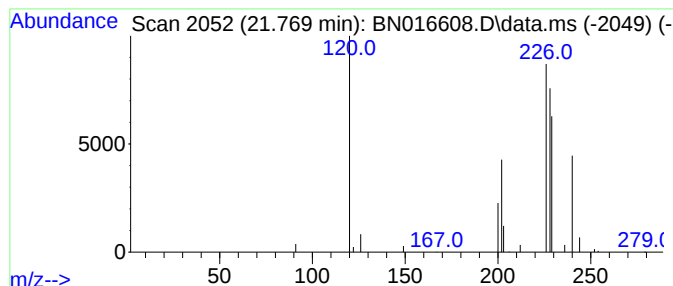
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cobalt, [(1,2,5,6-.eta.)-1,... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.769	0.67 ng	354242	Chrysene-d12	21.238

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cobalt, [(1,2,5,6-.eta.)-1,3,5,7...	228	C13H13Co	012110-49-5	9
2		Benzene, 1,2,4-trichloro-5-(meth...	226	C7H5Cl3S	004163-78-4	9
3		3-Bromo-7-methylbenzo(b)thiophene	226	C9H7BrS	001500-71-6	9
4		Aminoethylcysteine ketimine deca...	228	C9H12N2OS2	1000308-72-9	9
5		4-Amino-5-tert-butyl-4H-1,2,4-tr...	244	C9H20N4SSi	1000476-99-3	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Misc :
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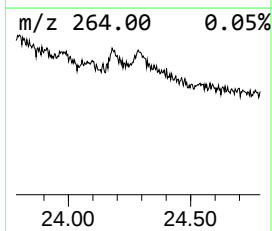
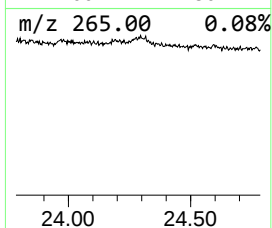
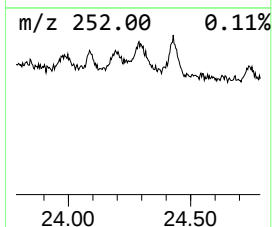
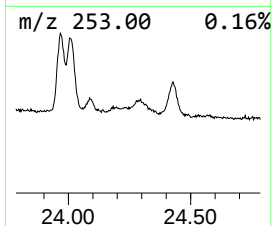
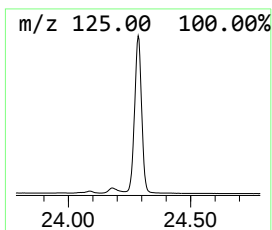
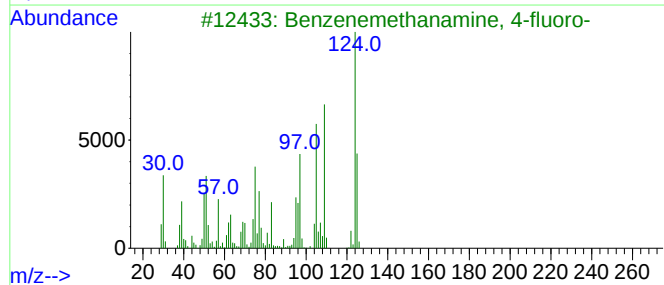
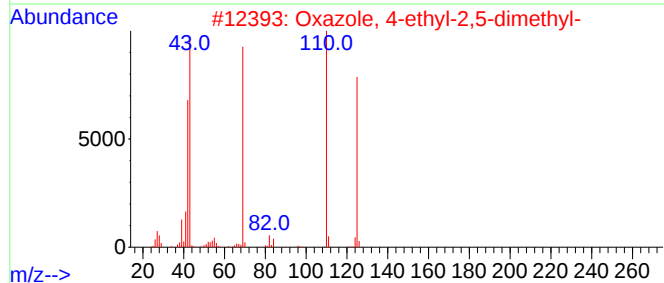
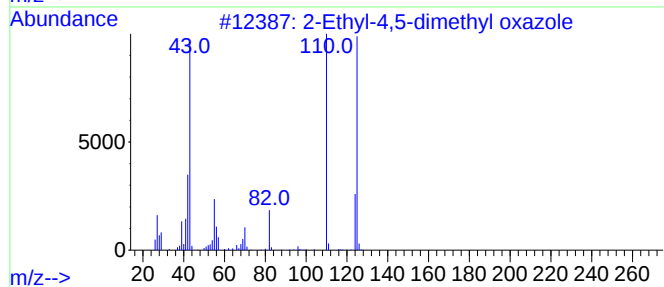
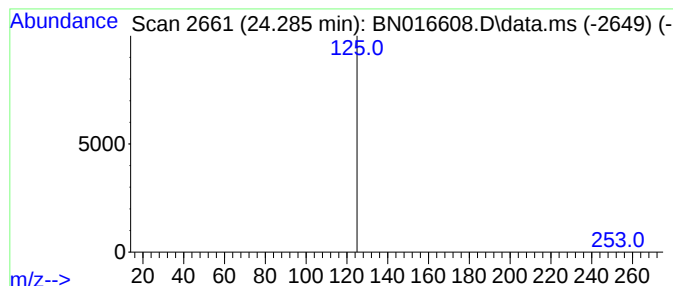
Instrument :
BNA_N
ClientSampleId :
UNDERPASS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2-Ethyl-4,5-dimethyl oxazole Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
24.285	0.26 ng	135497	Perylene-d12		23.484	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Ethyl-4,5-dimethyl oxazole		125	C7H11NO	053833-30-0	2
2	Oxazole, 4-ethyl-2,5-dimethyl-		125	C7H11NO	030408-61-8	2
3	Benzenemethanamine, 4-fluoro-		125	C7H8FN	000140-75-0	2
4	1-Butyl-1H-1,2,4-triazole		125	C6H11N3	006086-22-2	2
5	1H-Pyrrole-2,5-dione, 1-ethyl-		125	C6H7NO2	000128-53-0	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016608.D
Acq On : 30 Sep 2021 20:22
Operator : CG/JU
Sample : M3962-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
UNDERPASS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.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
Acetic acid, me...	3.816	0.1	ng	26747	1	7.642	95637	0.4
Ethene, (methyl...	3.908	0.4	ng	89064	1	7.642	95637	0.4
Butane	4.821	0.4	ng	85790	1	7.642	95637	0.4
1-Propanamine, ...	6.978	0.1	ng	12243	1	7.642	95637	0.4
2-Aminopropanen...	7.264	0.1	ng	14526	1	7.642	95637	0.4
Thiazolo[5,4-d]...	15.956	0.1	ng	42288	4	17.029	174614	0.4
6-[1-(1-Azepany...	16.384	0.0	ng	18412	4	17.029	174614	0.4
2,2-Diphenylpro...	17.954	0.0	ng	18086	4	17.029	174614	0.4
3-Hydroxy-2-pyr...	21.025	0.0	ng	22408	5	21.238	211414	0.4
Cobalt, [(1,2,5...	21.769	0.7	ng	354242	5	21.238	211414	0.4
2-Ethyl-4,5-dim...	24.285	0.3	ng	135497	6	23.484	208507	0.4