

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111623\
 Data File : BG059725.D
 Acq On : 16 Nov 2023 19:36
 Operator : MA/JU
 Sample : 05415-03
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RD-SW-01-20231103

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_G\Methods\8270-BG111623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG059725.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.731	222	228	236	rBV2	97081	166183	2.00%	0.291%
2	5.318	319	328	335	rBV	223268	411189	4.95%	0.720%
3	5.530	356	364	370	rBV	872524	1527155	18.37%	2.673%
4	5.835	409	416	429	rVB	303104	546525	6.57%	0.957%
5	6.452	514	521	525	rBV	205042	358751	4.32%	0.628%
6	6.517	525	532	537	rVV3	213349	463070	5.57%	0.811%
7	6.728	561	568	574	rBV	69491	126548	1.52%	0.222%
8	6.940	598	604	612	rVB4	97608	201600	2.43%	0.353%
9	7.093	624	630	637	rVB2	204872	362595	4.36%	0.635%
10	7.433	680	688	691	rBV2	359422	632690	7.61%	1.108%
11	7.469	691	694	700	rVB	228817	363561	4.37%	0.636%
12	7.586	708	714	722	rVB3	173349	293749	3.53%	0.514%
13	7.950	770	776	782	rVB3	186202	297019	3.57%	0.520%
14	8.338	837	842	845	rBV4	156604	293140	3.53%	0.513%
15	8.385	845	850	856	rVV2	395695	748868	9.01%	1.311%
16	8.526	867	874	879	rBV5	69997	140595	1.69%	0.246%
17	8.614	879	889	894	rBV3	248926	514849	6.19%	0.901%
18	8.726	901	908	911	rBV	135747	249410	3.00%	0.437%
19	8.773	911	916	922	rVV2	396104	673342	8.10%	1.179%
20	8.979	942	951	956	rBV8	64855	165457	1.99%	0.290%
21	9.120	967	975	979	rBV7	53291	145361	1.75%	0.254%
22	9.178	980	985	992	rVB5	93764	162762	1.96%	0.285%
23	9.272	992	1001	1004	rBV6	100659	229922	2.77%	0.402%
24	9.319	1005	1009	1015	rVB2	103580	183464	2.21%	0.321%
25	9.455	1024	1032	1038	rBV	1288282	2290543	27.55%	4.010%
26	9.543	1038	1047	1052	rBV	387875	712728	8.57%	1.248%
27	9.772	1074	1086	1090	rBV8	91218	200214	2.41%	0.350%
28	9.836	1091	1097	1102	rVV3	127540	272944	3.28%	0.478%
29	9.889	1102	1106	1113	rVB5	184445	306009	3.68%	0.536%
30	10.107	1139	1143	1154	rVB6	87750	204092	2.46%	0.357%
31	10.248	1160	1167	1174	rBV8	59151	164504	1.98%	0.288%
32	10.324	1174	1180	1182	rVV3	142795	255936	3.08%	0.448%
33	10.354	1182	1185	1194	rVB	178020	290149	3.49%	0.508%
34	10.630	1217	1232	1236	rBV2	117443	282978	3.40%	0.495%
35	10.788	1248	1259	1265	rBV8	82092	231635	2.79%	0.405%
36	10.947	1278	1286	1290	rVV2	82181	190763	2.29%	0.334%

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Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.017	1293	1298	1301	rVV5	96297	208685	2.51%	0.365%
38	11.070	1301	1307	1315	rVB2	1074397	1887343	22.70%	3.304%
39	11.194	1320	1328	1329	rBV	187651	318833	3.84%	0.558%
40	11.299	1340	1346	1354	rVB8	93033	224709	2.70%	0.393%
41	11.493	1371	1379	1390	rBV6	133133	394598	4.75%	0.691%
42	11.687	1407	1412	1420	rBV6	72520	174951	2.10%	0.306%
43	11.758	1420	1424	1430	rVB6	69108	146300	1.76%	0.256%
44	12.310	1511	1518	1524	rBV	601788	1003988	12.08%	1.757%
45	12.410	1531	1535	1545	rVB4	73994	153281	1.84%	0.268%
46	12.569	1555	1562	1569	rVB5	124676	243642	2.93%	0.426%
47	12.833	1598	1607	1612	rBV5	44696	130934	1.58%	0.229%
48	13.174	1656	1665	1671	rVV	1008808	1985809	23.89%	3.476%
49	13.244	1671	1677	1685	rVB	1346444	2064436	24.83%	3.614%
50	13.327	1685	1691	1697	rBV6	205174	325840	3.92%	0.570%
51	13.438	1705	1710	1721	rVB2	157878	361831	4.35%	0.633%
52	13.591	1726	1736	1749	rVB	1030233	1857393	22.34%	3.251%
53	14.114	1820	1825	1829	rBV5	127214	200619	2.41%	0.351%
54	14.302	1850	1857	1863	rBV	753971	1154692	13.89%	2.021%
55	14.419	1872	1877	1885	rBV	106061	304008	3.66%	0.532%
56	14.701	1921	1925	1934	rVB6	70496	145699	1.75%	0.255%
57	14.819	1937	1945	1950	rBV	446180	709134	8.53%	1.241%
58	14.966	1966	1970	1976	rVB2	241137	401655	4.83%	0.703%
59	15.083	1985	1990	1997	rVB	432918	635557	7.65%	1.113%
60	15.213	2006	2012	2018	rBV	661171	980999	11.80%	1.717%
61	15.471	2050	2056	2060	rBV	229301	366703	4.41%	0.642%
62	15.747	2099	2103	2108	rVB2	133462	201980	2.43%	0.354%
63	15.806	2108	2113	2119	rVB2	184802	263979	3.18%	0.462%
64	15.871	2119	2124	2127	rBV3	91441	152248	1.83%	0.267%
65	16.047	2146	2154	2167	rVB	5472311	8312983	100.00%	14.552%
66	16.317	2195	2200	2208	rVB	323992	590509	7.10%	1.034%
67	16.470	2220	2226	2232	rVB	820158	1345016	16.18%	2.354%
68	16.681	2259	2262	2270	rVB	120921	219836	2.64%	0.385%
69	16.981	2308	2313	2320	rBV	314557	509720	6.13%	0.892%
70	17.093	2328	2332	2340	rVB4	156420	238257	2.87%	0.417%
71	17.234	2351	2356	2361	rBV	405810	588971	7.08%	1.031%
72	17.686	2429	2433	2435	rVV3	102773	162440	1.95%	0.284%
73	17.721	2435	2439	2445	rVV2	334812	687287	8.27%	1.203%
74	17.774	2445	2448	2453	rVB4	210169	316794	3.81%	0.555%
75	17.974	2477	2482	2489	rVB5	160136	309041	3.72%	0.541%
76	18.168	2511	2515	2525	rBV4	91676	198061	2.38%	0.347%

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77	18.421	2554	2558	2567	rVB5	99858	187843	2.26%	0.329%
78	18.538	2575	2578	2583	rVB4	161956	200999	2.42%	0.352%
79	18.685	2599	2603	2608	rBV4	126587	190738	2.29%	0.334%
80	18.908	2636	2641	2649	rVV6	268461	484020	5.82%	0.847%
81	20.113	2842	2846	2850	rBV2	187971	278684	3.35%	0.488%
82	20.295	2871	2877	2882	rVV	1990787	2439661	29.35%	4.271%
83	20.377	2886	2891	2897	rBV10	54706	132725	1.60%	0.232%
84	21.106	3009	3015	3021	rVB10	62475	136700	1.64%	0.239%
85	21.458	3070	3075	3077	rBV4	104120	154348	1.86%	0.270%
86	21.493	3078	3081	3087	rVB5	123661	219354	2.64%	0.384%
87	21.611	3094	3101	3104	rBV9	83055	190940	2.30%	0.334%
88	22.040	3168	3174	3182	rBV	310680	674550	8.11%	1.181%
89	22.151	3190	3193	3198	rVB7	95512	155045	1.87%	0.271%
90	22.574	3259	3265	3279	rVB6	183437	556196	6.69%	0.974%
91	23.285	3382	3386	3399	rVB7	176910	435472	5.24%	0.762%
92	23.426	3407	3410	3414	rBV5	59357	129276	1.56%	0.226%
93	23.479	3414	3419	3428	rVB2	257293	581674	7.00%	1.018%
94	23.691	3449	3455	3462	rBV8	72605	174479	2.10%	0.305%
95	24.566	3596	3604	3617	rVB3	284555	838907	10.09%	1.469%
96	25.630	3776	3785	3798	rBV3	176229	606975	7.30%	1.063%
97	25.900	3821	3831	3841	rBV4	302007	994921	11.97%	1.742%
98	27.580	4103	4117	4126	rBV7	211233	864627	10.40%	1.514%
99	29.672	4456	4473	4486	rBV8	206072	1128178	13.57%	1.975%
100	32.304	4910	4921	4922	rBV9	97945	230891	2.78%	0.404%

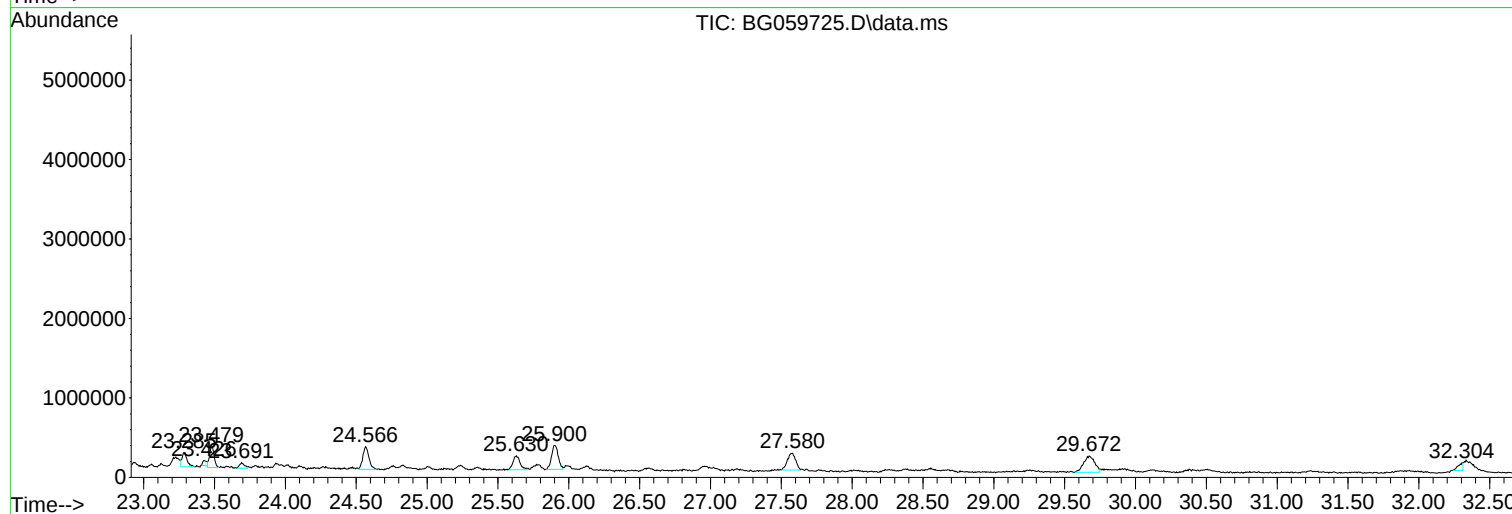
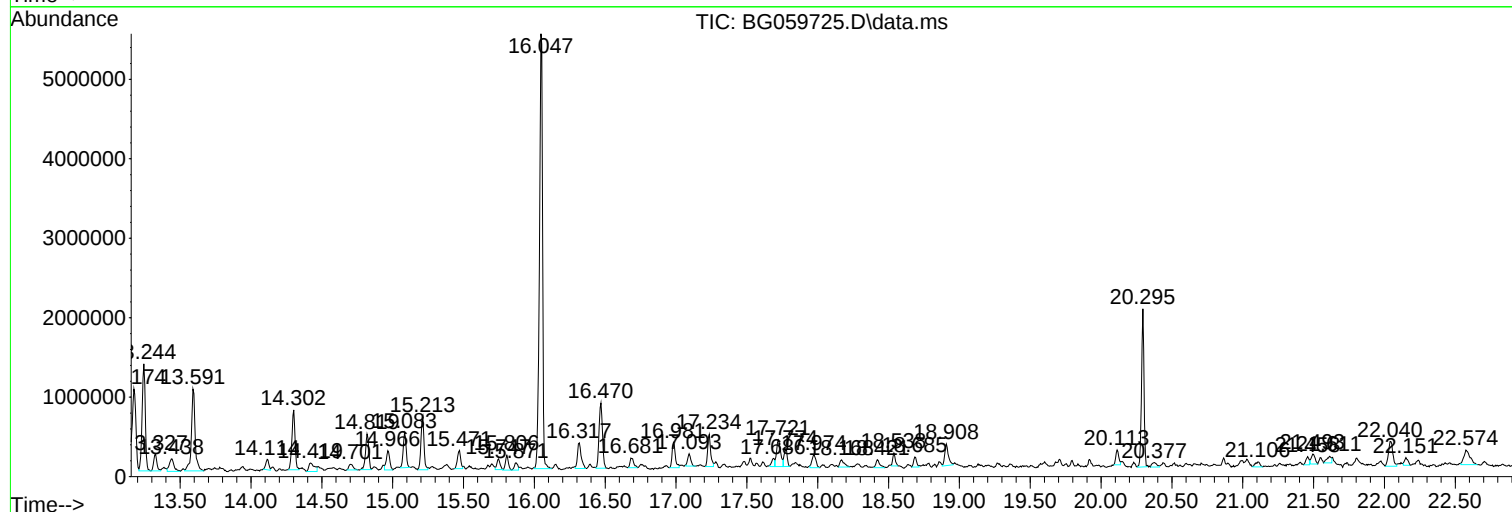
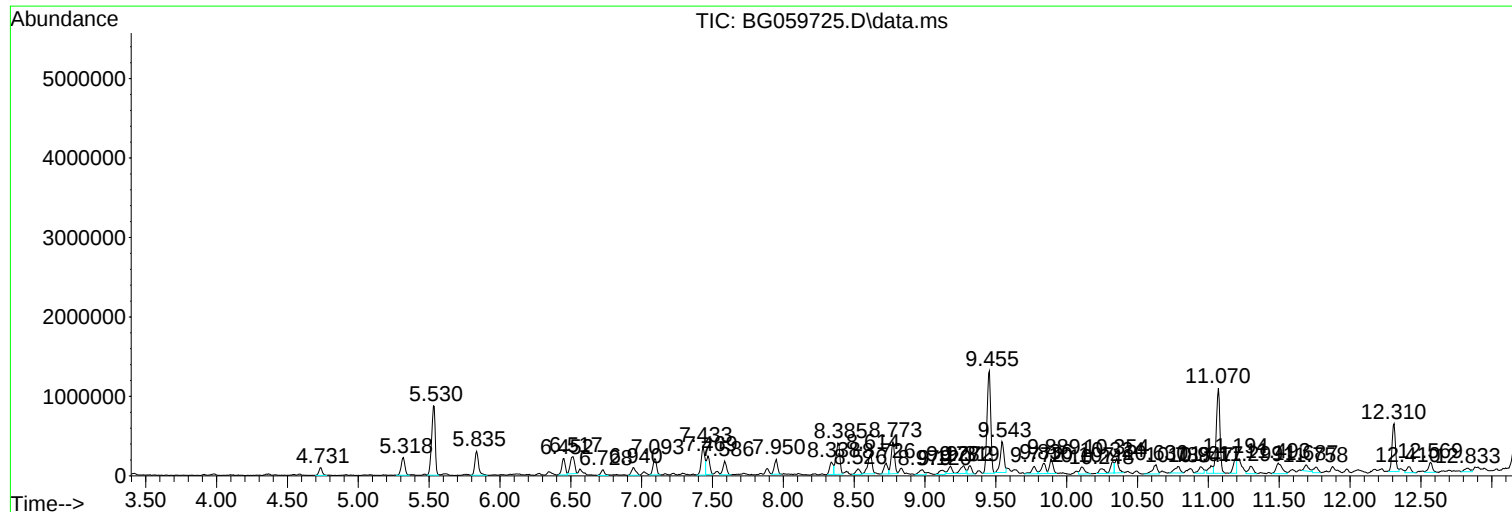
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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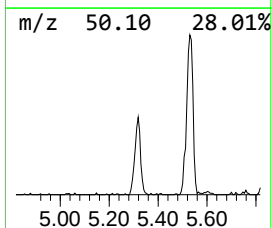
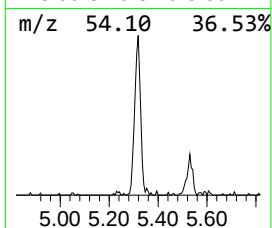
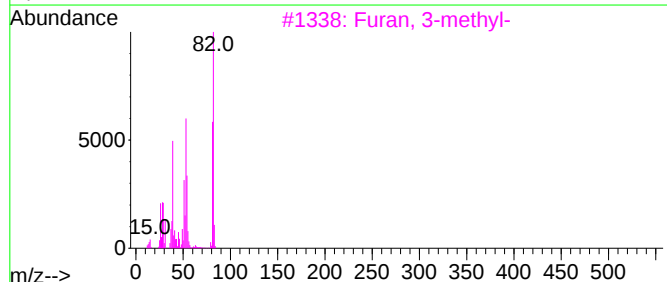
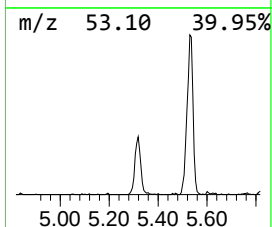
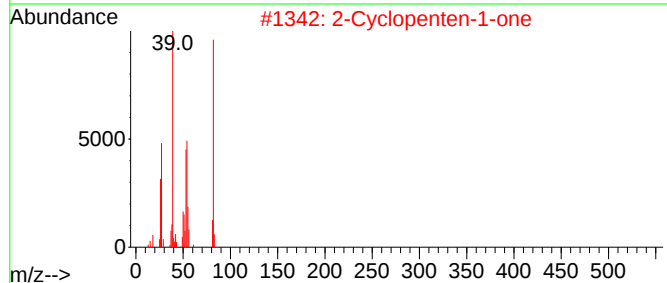
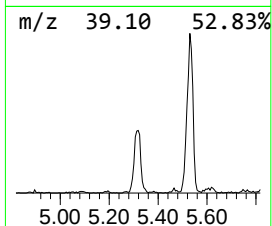
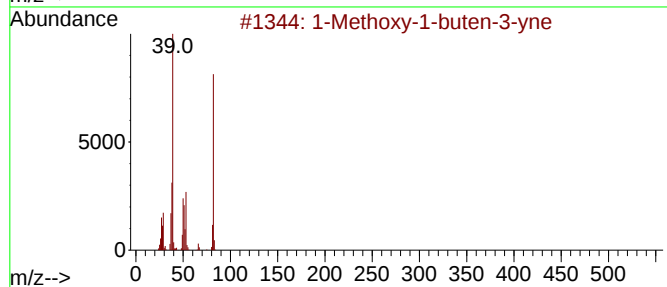
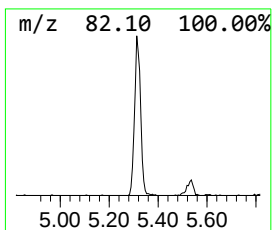
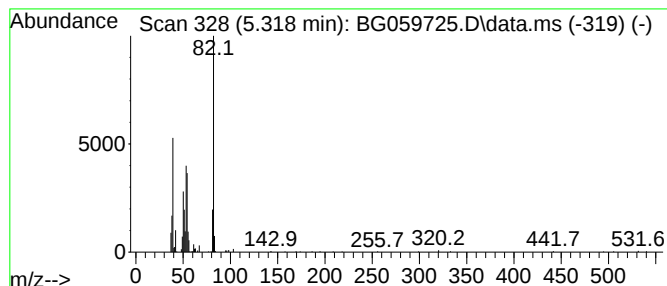
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Methoxy-1-buten-3-yne Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.318	28.05 ng	411189	1,4-Dichlorobenzene-d4	8.344

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Methoxy-1-buten-3-yne	82	C5H6O	002798-73-4	90
2			2-Cyclopenten-1-one	82	C5H6O	000930-30-3	78
3			Furan, 3-methyl-	82	C5H6O	000930-27-8	59
4			2,5-Furandione, 3,4-dimethyl-	126	C6H6O3	000766-39-2	56
5			3-Cyclobutene-1,2-dione, 3,4-dim...	110	C6H6O2	001121-15-9	50



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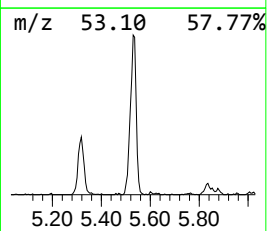
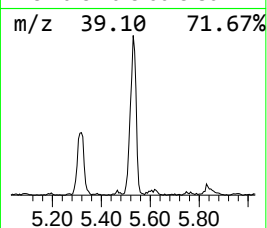
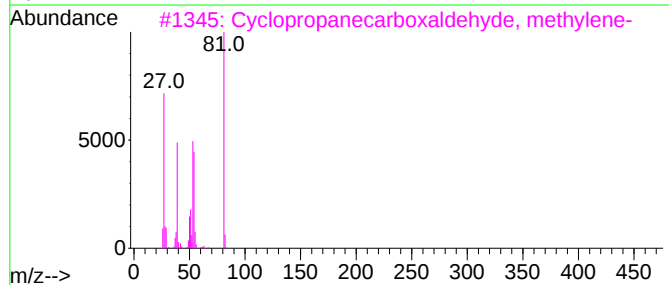
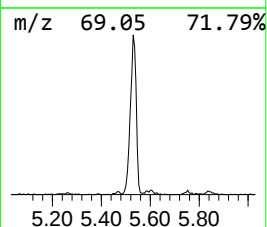
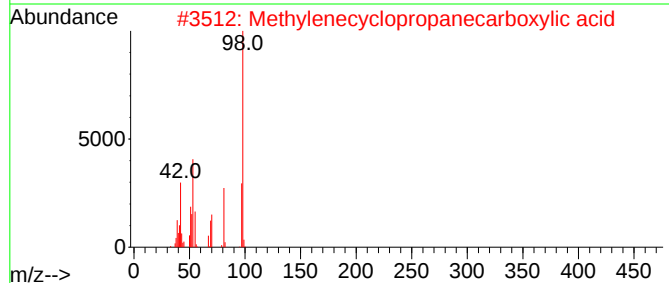
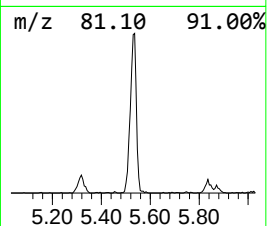
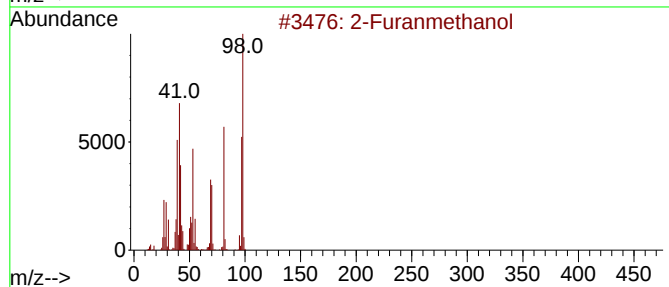
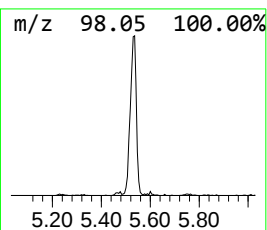
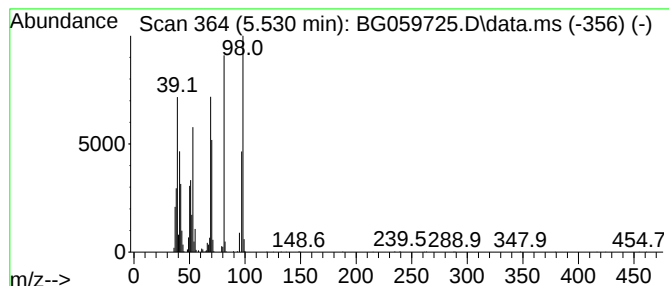
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Furanmethanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.530	104.19 ng	1527160	1,4-Dichlorobenzene-d4	8.344

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Furanmethanol	98	C5H6O2	000098-00-0	70
2			Methylenecyclopropanecarboxylic ...	98	C5H6O2	062266-36-8	38
3			Cyclopropanecarboxaldehyde, meth...	82	C5H6O	142423-24-3	38
4			2-Butyn-1-ol	70	C4H6O	000764-01-2	37
5			Guanosine, 2'-deoxy-6-thio-	283	C10H13N5O3S	000789-61-7	36



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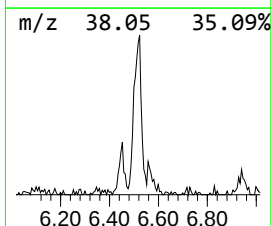
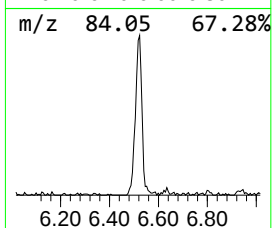
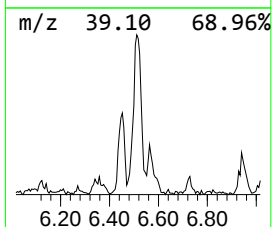
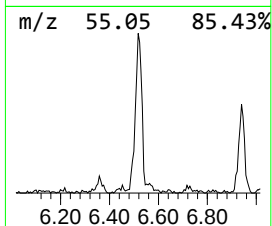
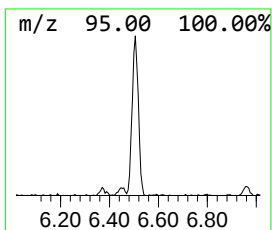
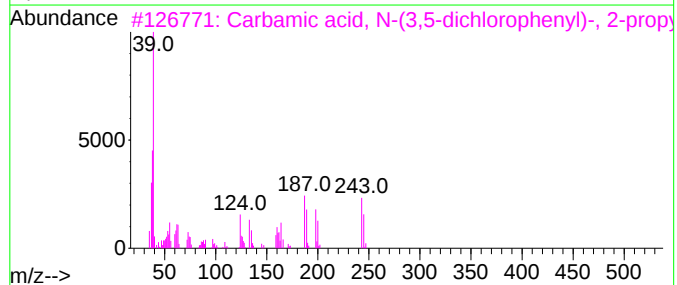
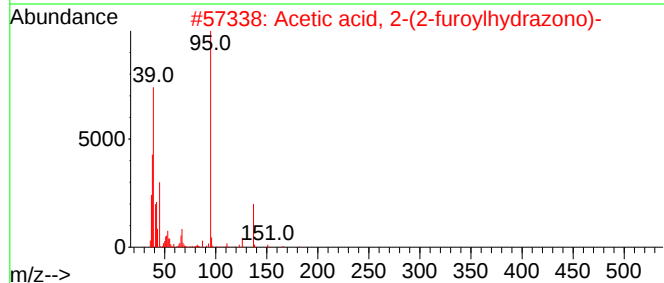
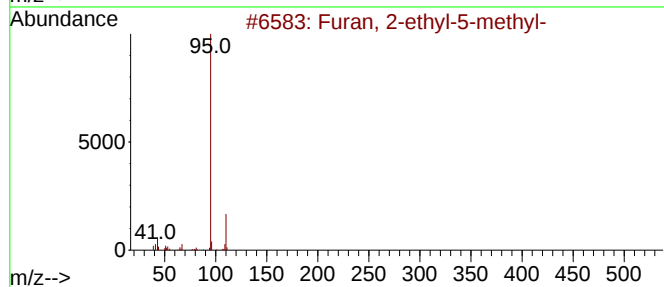
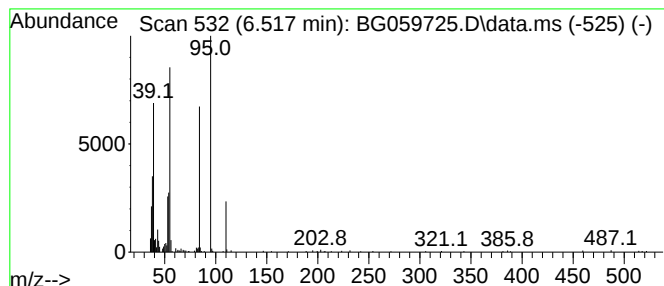
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.517 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.517	31.59 ng	463070	1,4-Dichlorobenzene-d4	8.344

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, 2-ethyl-5-methyl-	110	C7H10O	001703-52-2	43
2			Acetic acid, 2-(2-furoylhydrazono)-	182	C7H6N2O4	139397-87-8	36
3			Carbamic acid, N-(3,5-dichlorophenyl)-, 2-propyl-	243	C10H7Cl2NO2	025216-52-8	35
4			2(5H)-Furanone	84	C4H4O2	000497-23-4	25
5			Cyclopropene	40	C3H4	002781-85-3	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111623\
Data File : BG059725.D
Acq On : 16 Nov 2023 19:36
Operator : MA/JU
Sample : 05415-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

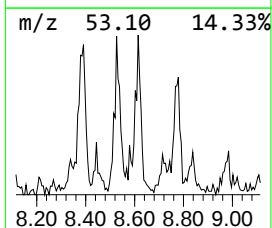
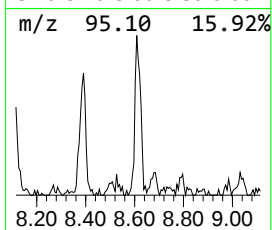
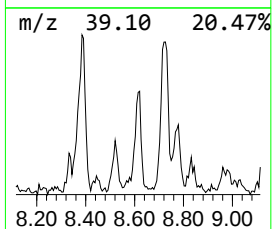
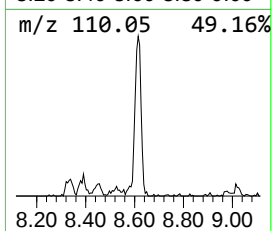
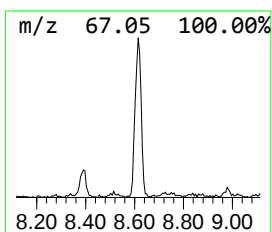
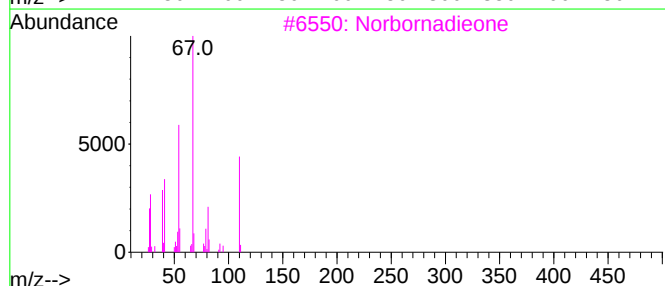
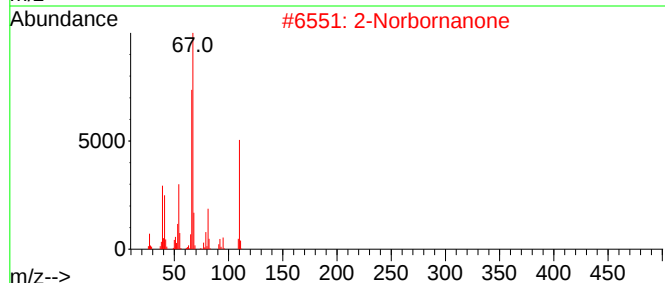
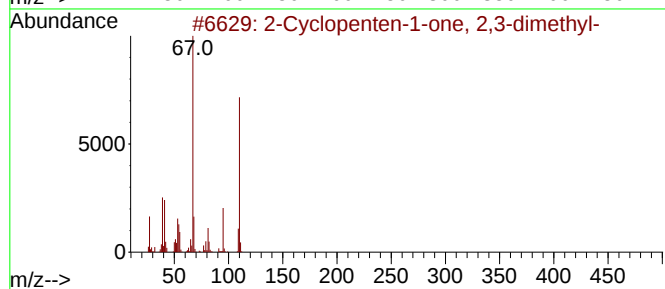
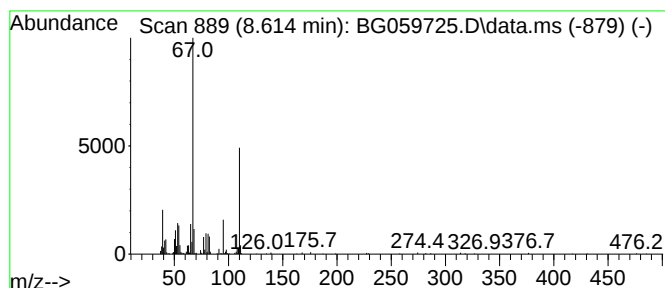
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 2-Cyclopenten-1-one, 2,3-di... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD			R.T.
8.614	35.13 ng	514849	1,4-Dichlorobenzene-d4			8.344
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Cyclopenten-1-one, 2,3-dimethyl-		110	C7H10O	001121-05-7	87
2	2-Norbornanone		110	C7H10O	000497-38-1	72
3	Norbornadieone		110	C7H10O	010218-02-7	72
4	1,4-Pentadiene, 2-methyl-		82	C6H10	000763-30-4	49
5	1,4-Pentadiene, 3-methyl-		82	C6H10	001115-08-8	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111623\
Data File : BG059725.D
Acq On : 16 Nov 2023 19:36
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Sample : 05415-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

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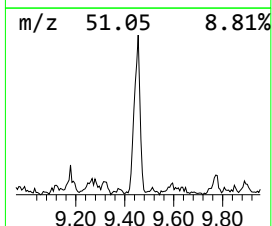
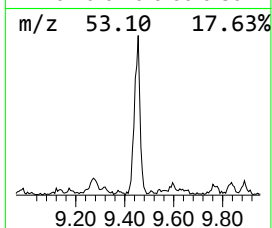
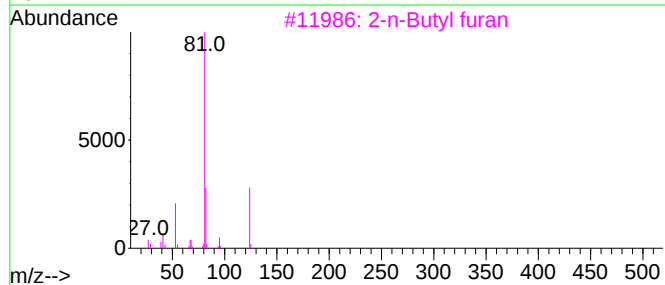
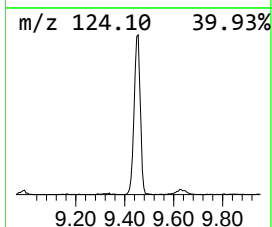
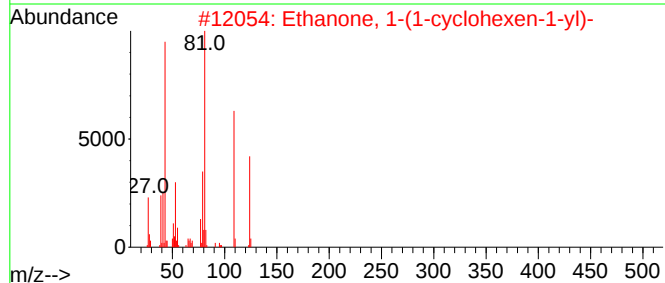
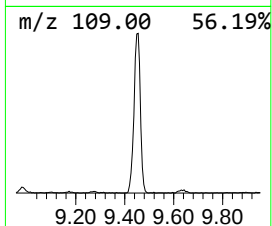
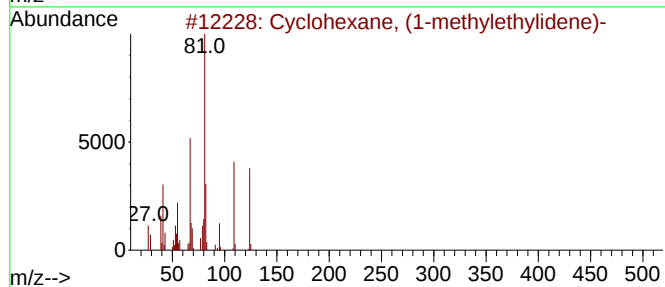
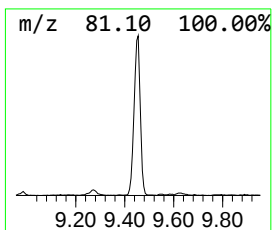
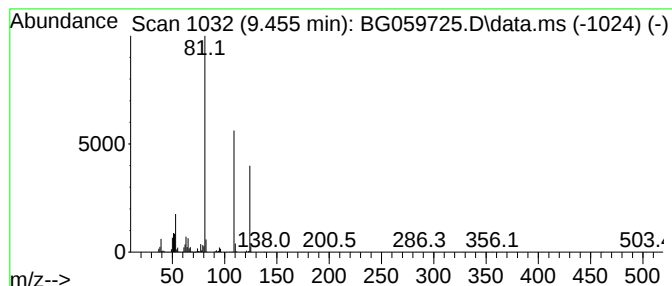
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Cyclohexane, (1-methylethyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.455	156.28 ng	2290540	1,4-Dichlorobenzene-d4	8.344

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, (1-methylethylidene)-	124	C9H16	005749-72-4	74
2			Ethanone, 1-(1-cyclohexen-1-yl)-	124	C8H12O	000932-66-1	59
3			2-n-Butyl furan	124	C8H12O	004466-24-4	53
4			Mequinol	124	C7H8O2	000150-76-5	46
5			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111623\
Data File : BG059725.D
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Sample : 05415-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

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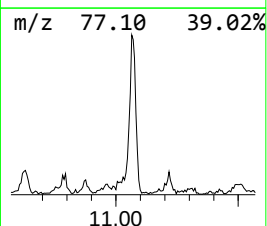
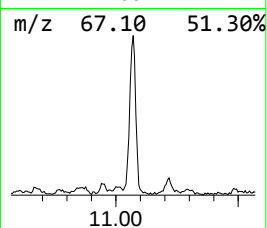
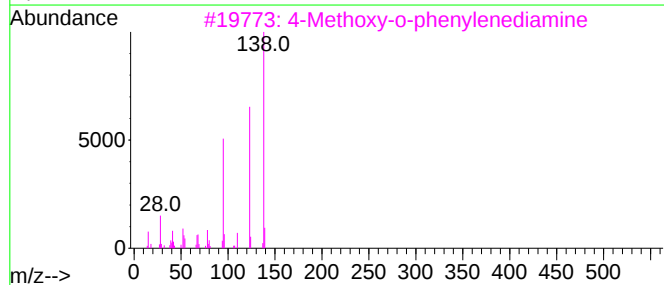
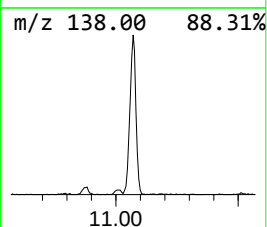
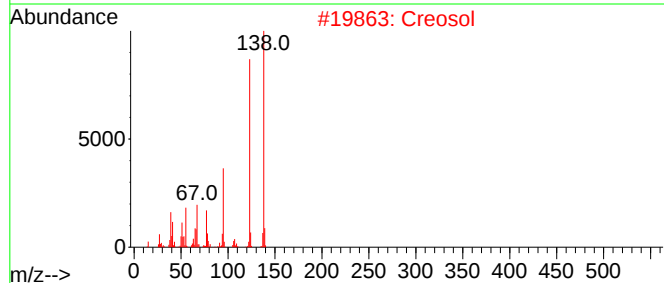
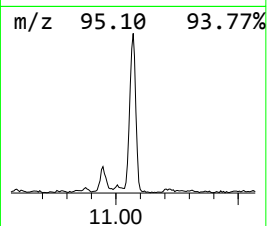
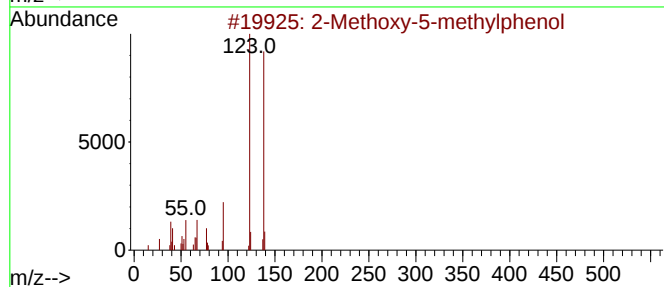
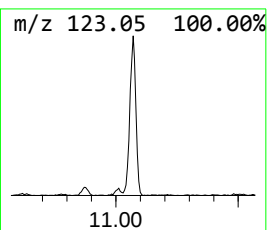
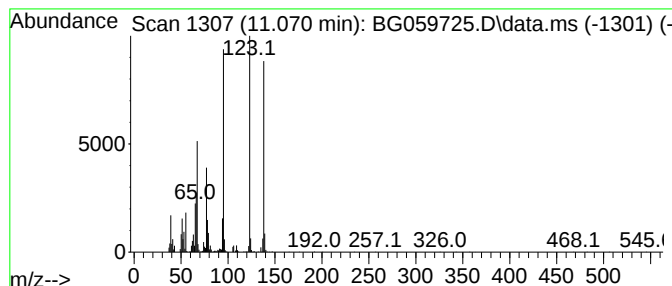
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-Methoxy-5-methylphenol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.070	118.39 ng	1887340	Naphthalene-d8	11.188

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methoxy-5-methylphenol	138	C8H10O2	001195-09-1	90
2			Creosol	138	C8H10O2	000093-51-6	74
3			4-Methoxy-o-phenylenediamine	138	C7H10N2O	000102-51-2	49
4			4-Acetyl-1-methylcyclohexene	138	C9H14O	006090-09-1	49
5			2-Methoxy-p-phenylenediamine	138	C7H10N2O	1000237-93-1	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111623\
Data File : BG059725.D
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Sample : 05415-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

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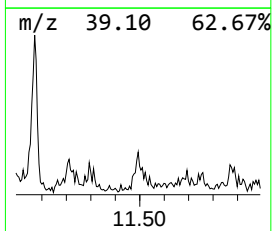
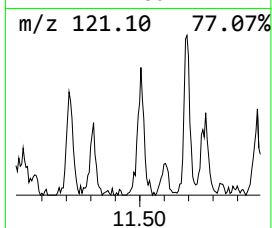
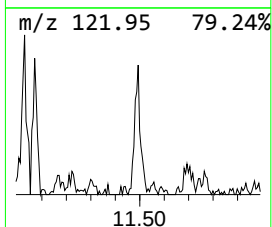
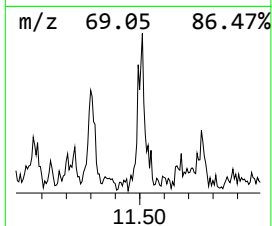
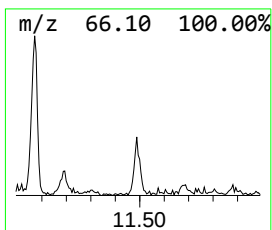
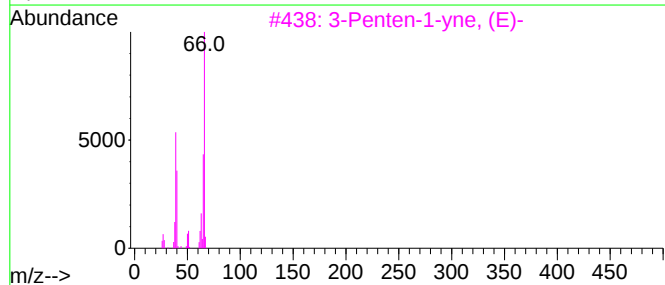
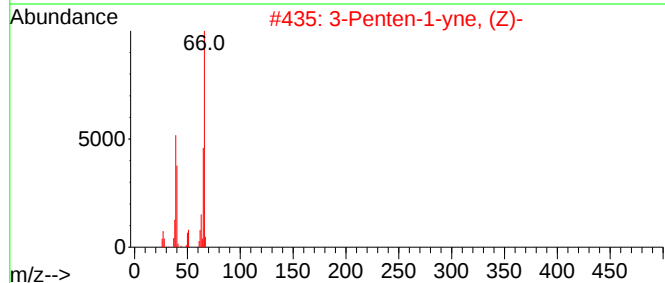
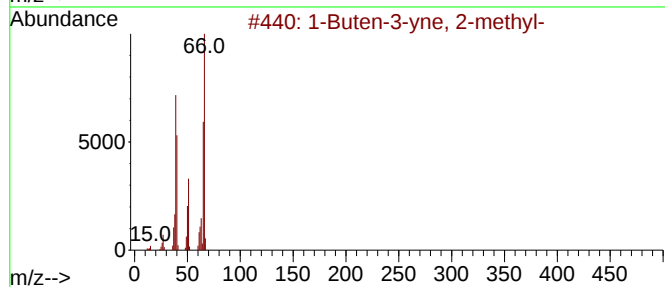
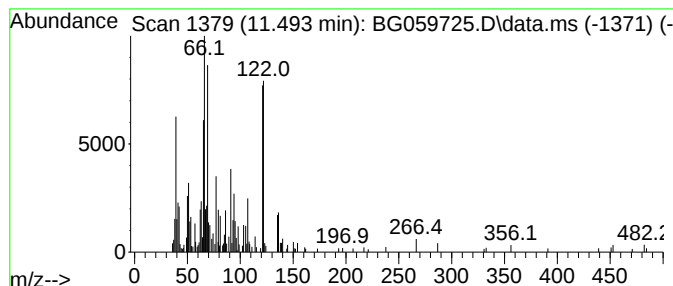
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown11.493 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.493	24.75 ng	394598	Naphthalene-d8	11.188

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Buten-3-yne, 2-methyl-	66	C5H6	000078-80-8	49
2			3-Penten-1-yne, (Z)-	66	C5H6	001574-40-9	46
3			3-Penten-1-yne, (E)-	66	C5H6	002004-69-5	46
4			1(2H)-Pentalenone, 3,3a,4,6a-tet...	122	C8H10O	056138-05-7	43
5			Cyclopropylacetylene	66	C5H6	006746-94-7	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111623\
Data File : BG059725.D
Acq On : 16 Nov 2023 19:36
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ClientSampleId :
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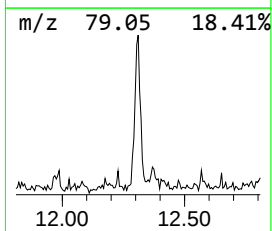
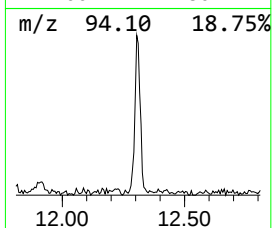
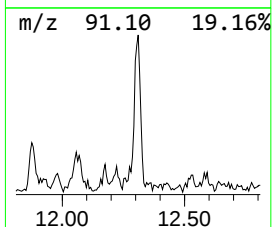
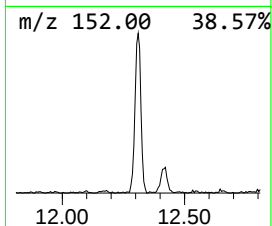
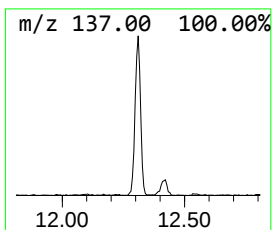
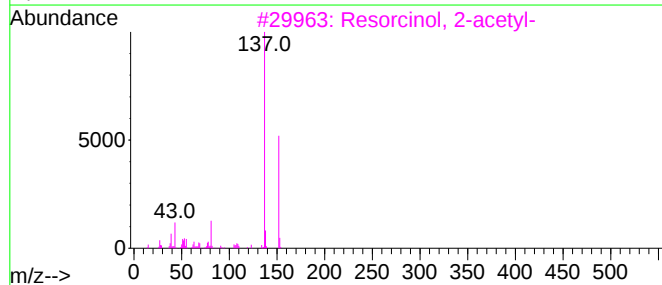
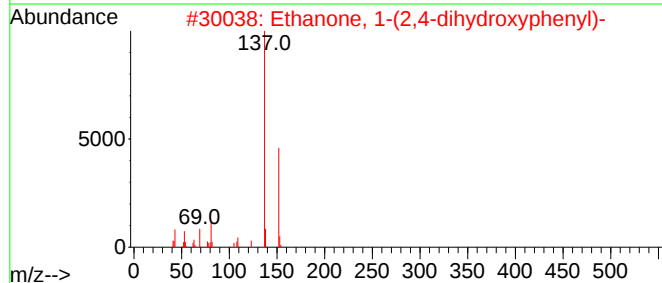
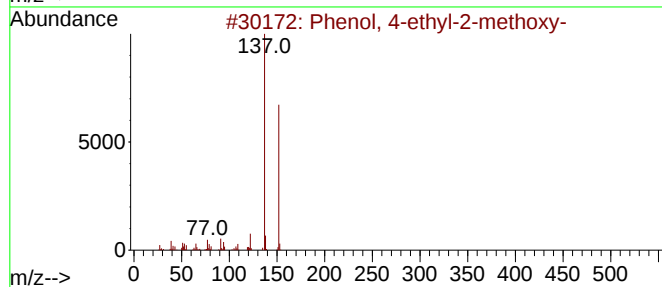
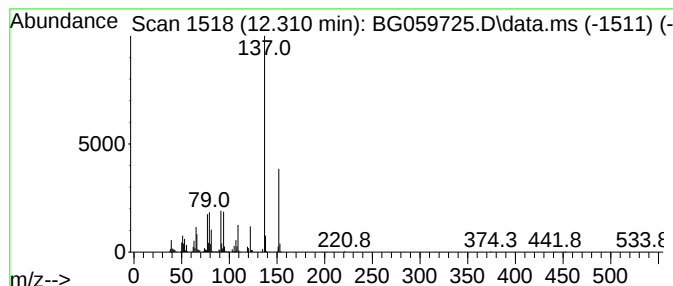
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Phenol, 4-ethyl-2-methoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.310	62.98 ng	1003990	Naphthalene-d8	11.188

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4-ethyl-2-methoxy-	152	C9H12O2	002785-89-9	90
2			Ethanone, 1-(2,4-dihydroxyphenyl)-	152	C8H8O3	000089-84-9	74
3			Resorcinol, 2-acetyl-	152	C8H8O3	000699-83-2	72
4			1-(2,3-Dihydroxyphenyl)ethanone	152	C8H8O3	1000434-39-0	72
5			O-Methoxy-.alpha.-methylbenzyl a...	152	C9H12O2	013513-82-1	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111623\
Data File : BG059725.D
Acq On : 16 Nov 2023 19:36
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ClientSampleId :
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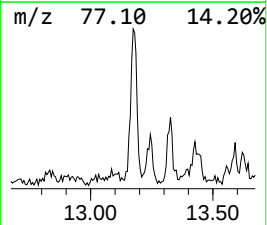
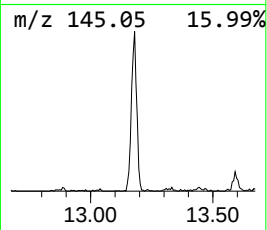
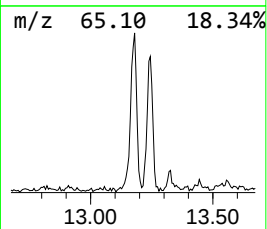
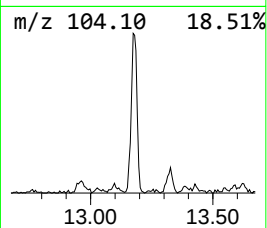
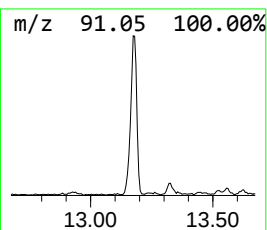
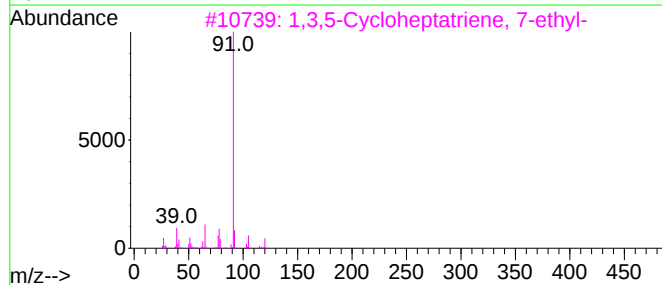
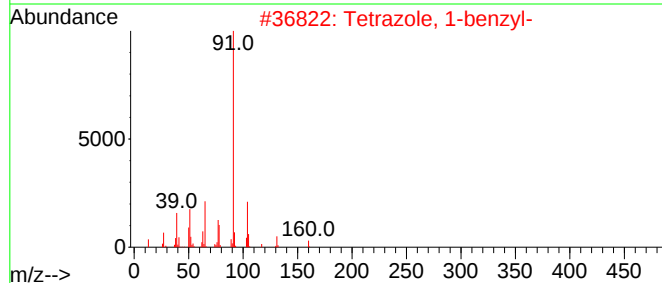
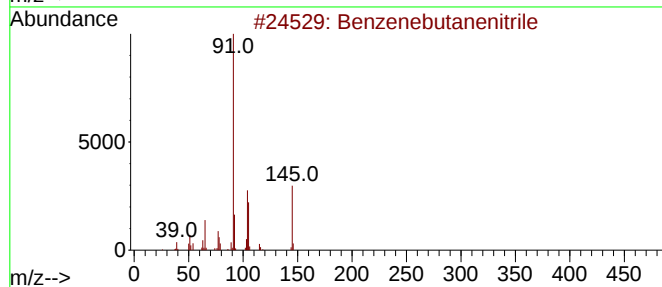
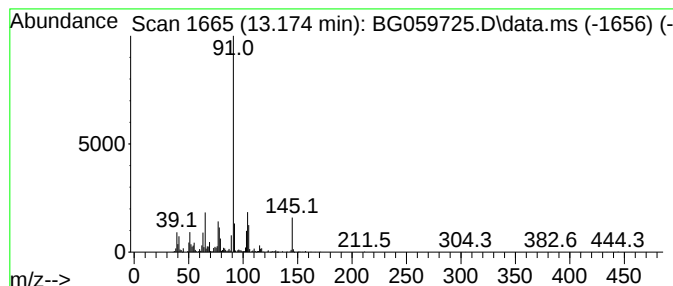
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzenebutanenitrile Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.174	98.88 ng	1985810	Acenaphthene-d10	14.966

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenebutanenitrile	145	C10H11N	002046-18-6	72
2			Tetrazole, 1-benzyl-	160	C8H8N4	006926-50-7	53
3			1,3,5-Cycloheptatriene, 7-ethyl-	120	C9H12	017634-51-4	50
4			Cyclopropylphenylmethane	132	C10H12	001667-00-1	50
5			N-(Benzyloxy)-2,2,2-trifluoroace...	219	C9H8F3NO2	174075-91-3	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111623\
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Acq On : 16 Nov 2023 19:36
Operator : MA/JU
Sample : 05415-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
RD-SW-01-20231103

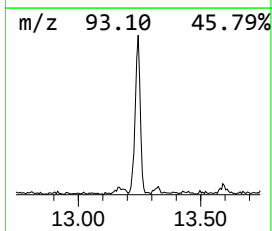
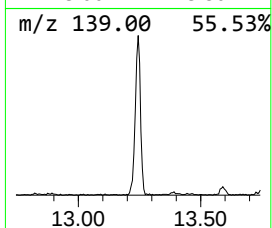
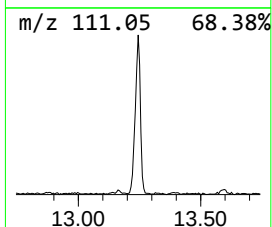
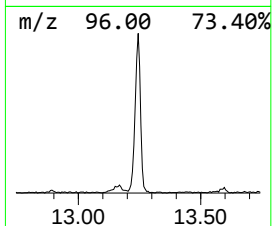
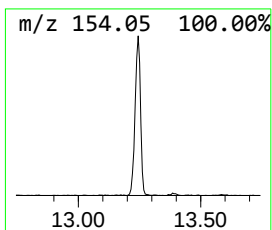
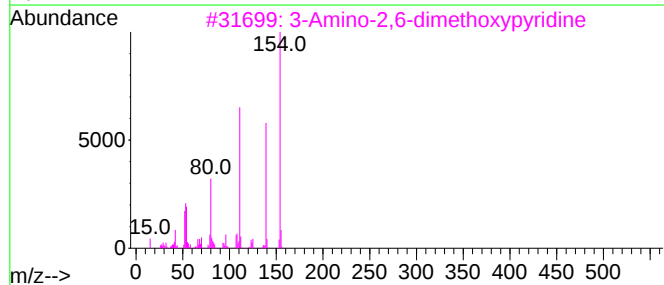
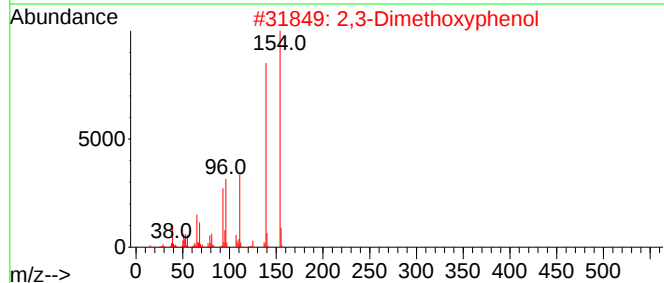
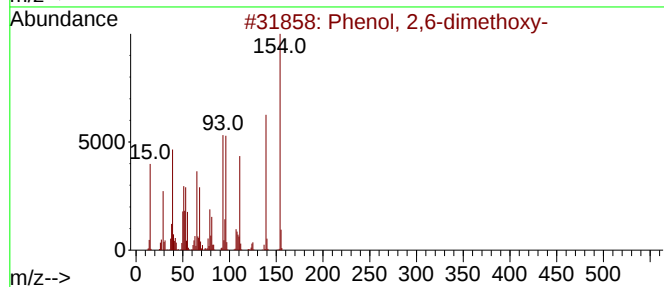
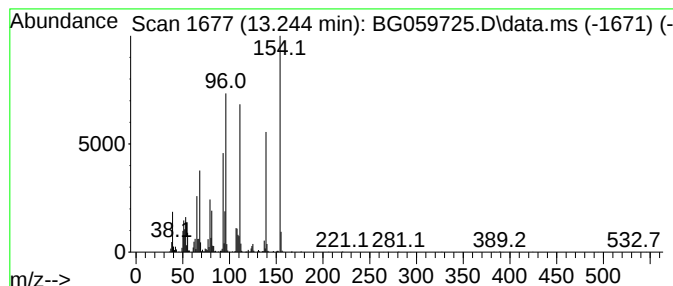
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Phenol, 2,6-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.244	102.80 ng	2064440	Acenaphthene-d10	14.966

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,6-dimethoxy-	154	C8H10O3	000091-10-1	81
2			2,3-Dimethoxyphenol	154	C8H10O3	005150-42-5	64
3			3-Amino-2,6-dimethoxypyridine	154	C7H10N2O2	028020-37-3	49
4			2(3H)-Furanone, 3-(dihydro-2(3H)...	154	C8H10O3	055164-40-4	43
5			Phenol, 3-methyl-4-(methylthio)-	154	C8H10OS	003120-74-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111623\
Data File : BG059725.D
Acq On : 16 Nov 2023 19:36
Operator : MA/JU
Sample : 05415-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
RD-SW-01-20231103

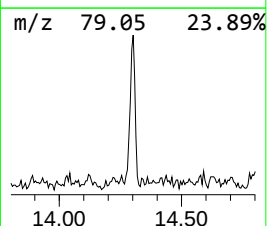
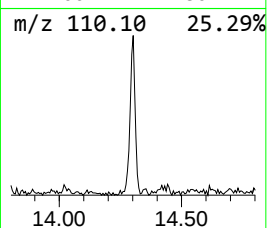
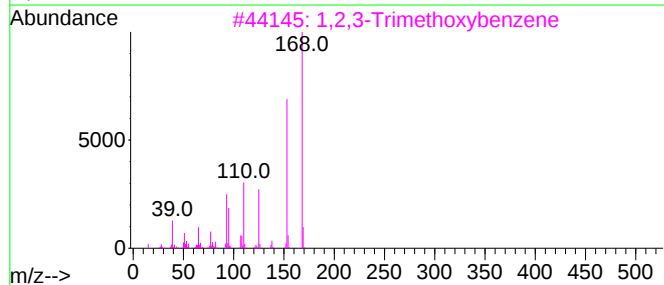
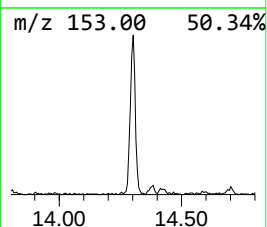
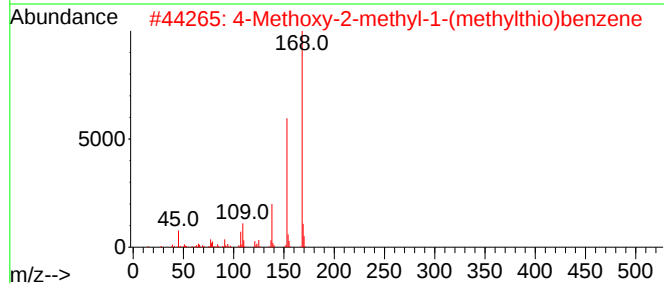
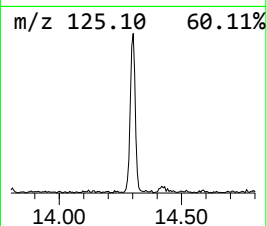
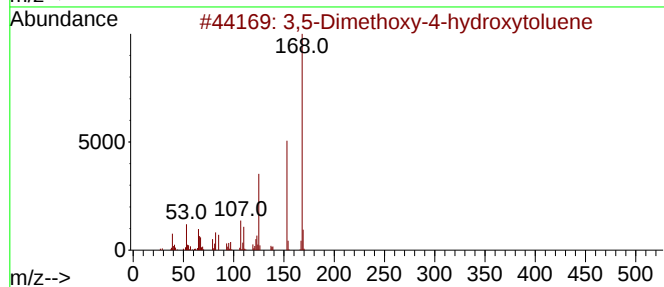
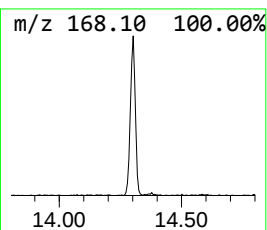
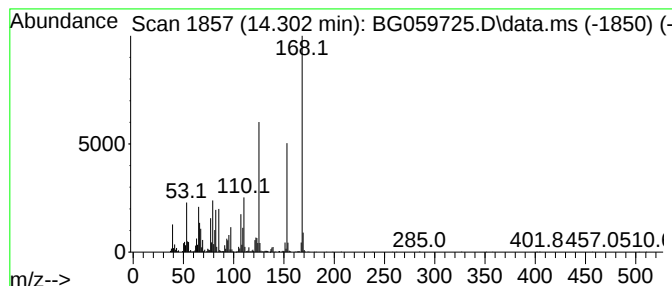
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown14.302 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.302	57.50 ng	1154690	Acenaphthene-d10	14.966

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,5-Dimethoxy-4-hydroxytoluene	168	C9H12O3	006638-05-7	49
2			4-Methoxy-2-methyl-1-(methylthio)benzene	168	C9H12OS	022583-04-6	43
3			1,2,3-Trimethoxybenzene	168	C9H12O3	000634-36-6	43
4			Benzenamine, 2-methoxy-4-nitro-	168	C7H8N2O3	000097-52-9	38
5			2,5-Dimethoxybenzyl alcohol	168	C9H12O3	033524-31-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111623\
Data File : BG059725.D
Acq On : 16 Nov 2023 19:36
Operator : MA/JU
Sample : 05415-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

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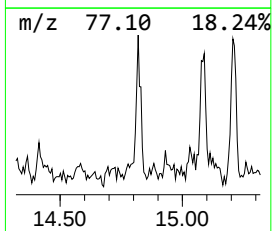
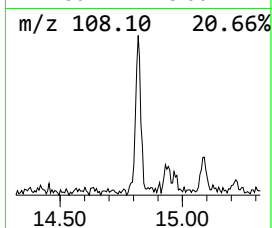
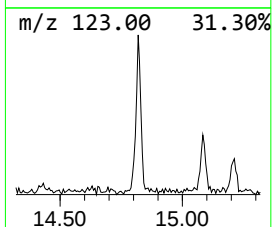
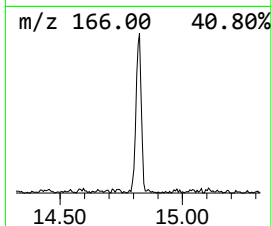
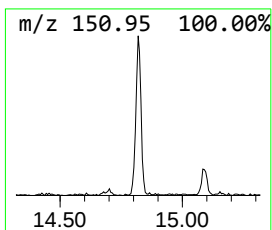
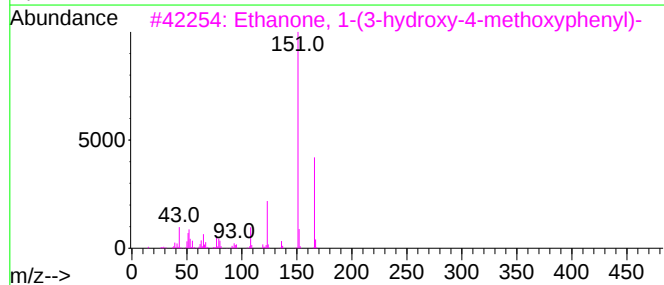
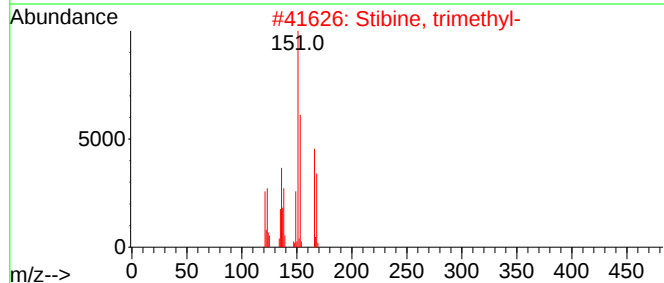
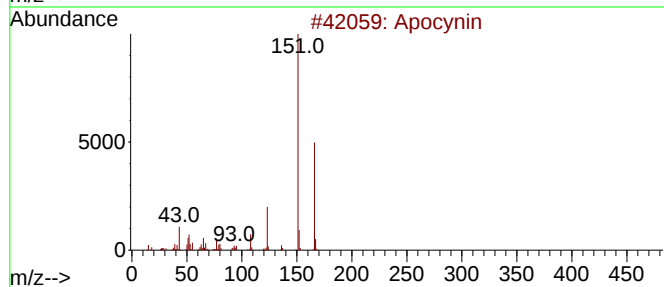
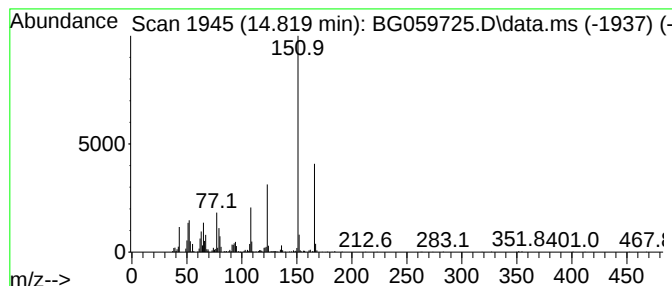
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Apocynin Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.819	35.31 ng	709134	Acenaphthene-d10	14.966

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Apocynin			166	C9H10O3	000498-02-2	91
2	Stibine, trimethyl-			166	C3H9Sb	000594-10-5	83
3	Ethanone, 1-(3-hydroxy-4-methoxy...			166	C9H10O3	006100-74-9	72
4	1-(2-Hydroxy-3-methoxyphenyl)eth...			166	C9H10O3	1000434-39-1	64
5	Ethanone, 1-(2-hydroxy-6-methoxy...			166	C9H10O3	000703-23-1	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111623\
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Operator : MA/JU
Sample : 05415-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

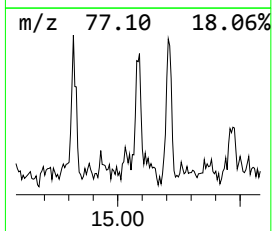
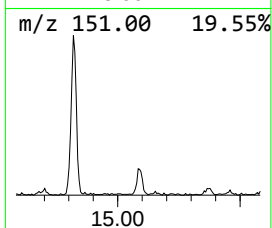
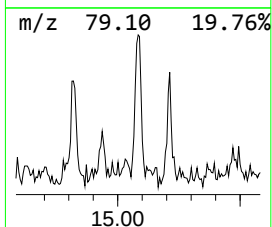
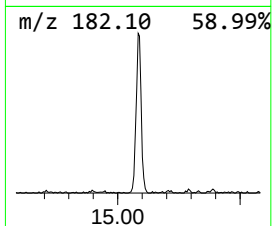
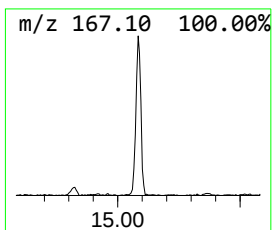
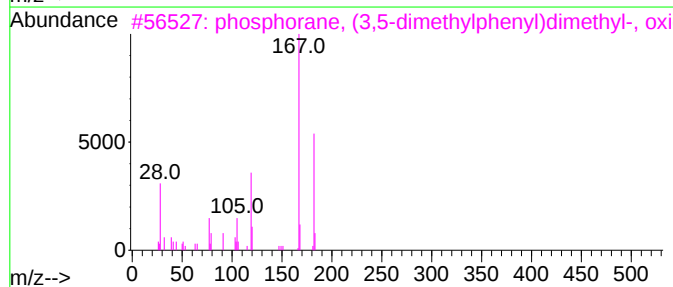
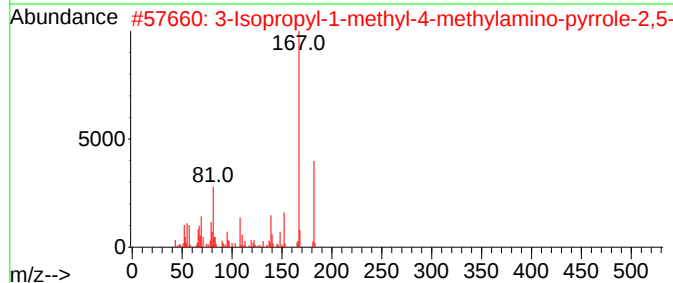
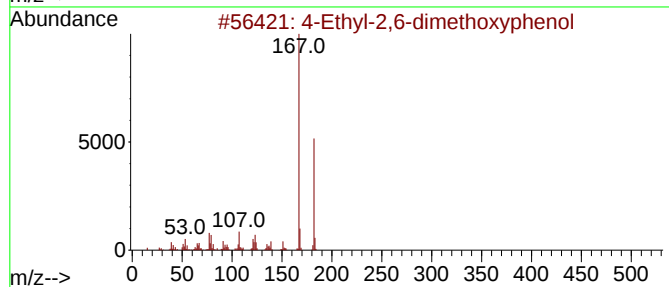
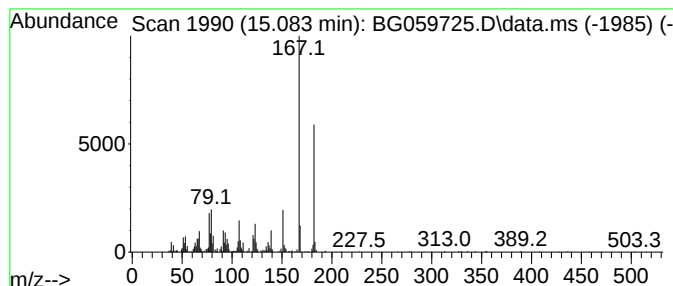
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 4-Ethyl-2,6-dimethoxyphenol Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.083	31.65 ng	635557	Acenaphthene-d10	14.966	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Ethyl-2,6-dimethoxyphenol	182	C10H14O3	014059-92-8	76
2	3-Isopropyl-1-methyl-4-methylami...	182	C9H14N2O2	1000296-12-2	53
3	phosphorane, (3,5-dimethylphenyl...	182	C10H15OP	1000404-87-3	52
4	Ethanone, 1-(2,6-dihydroxy-4-met...	182	C9H10O4	007507-89-3	50
5	2,5-Dimethoxybenzoic acid	182	C9H10O4	002785-98-0	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111623\
Data File : BG059725.D
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Operator : MA/JU
Sample : 05415-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

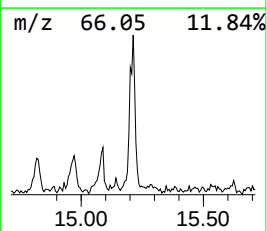
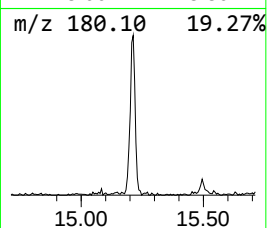
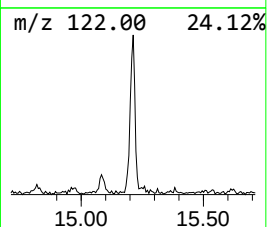
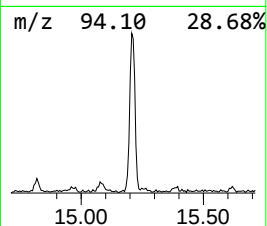
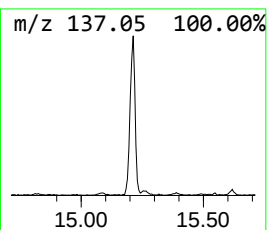
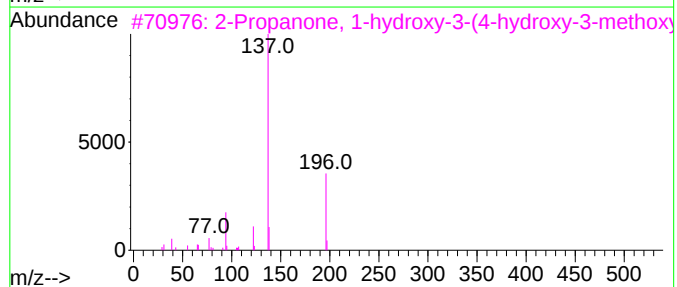
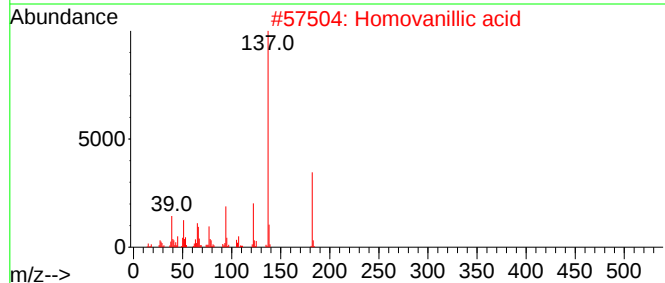
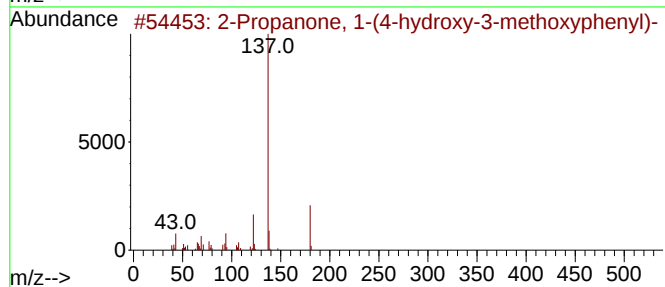
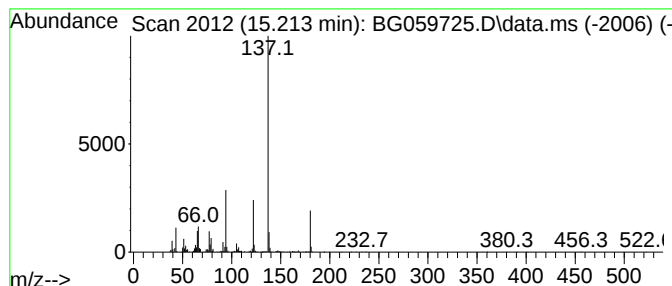
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 2-Propanone, 1-(4-hydroxy-3... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.213	48.85 ng	980999	Acenaphthene-d10	14.966	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanone, 1-(4-hydroxy-3-meth...	180	C10H12O3	002503-46-0	86
2	Homovanillic acid	182	C9H10O4	000306-08-1	64
3	2-Propanone, 1-hydroxy-3-(4-hydr...	196	C10H12O4	004899-74-5	59
4	1-(4-methylthiophenyl)-2-propanone	180	C10H12OS	1000378-99-8	58
5	Homovanillyl alcohol	168	C9H12O3	002380-78-1	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111623\
Data File : BG059725.D
Acq On : 16 Nov 2023 19:36
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ClientSampleId :
RD-SW-01-20231103

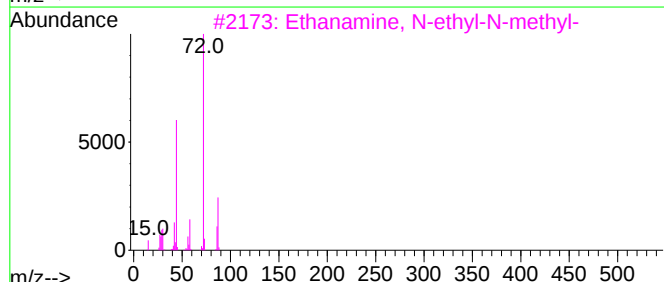
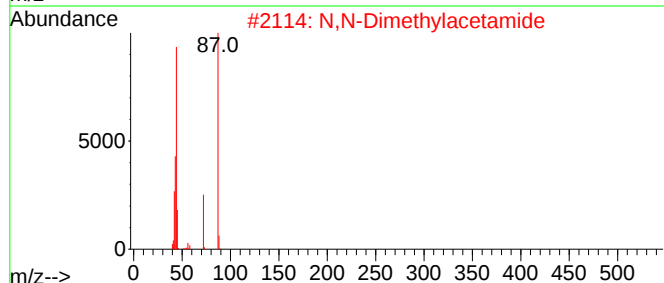
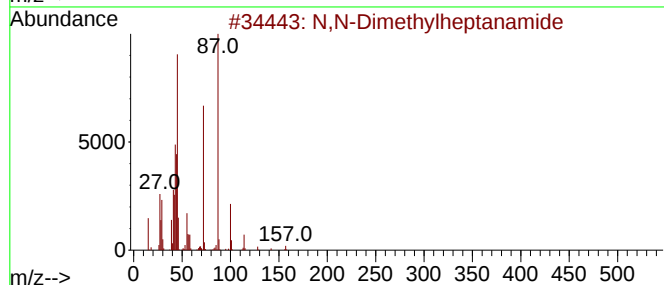
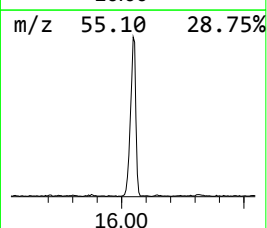
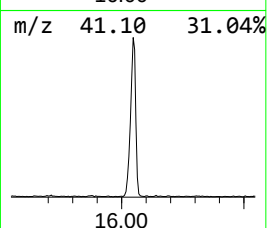
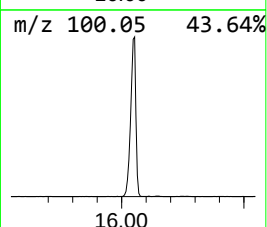
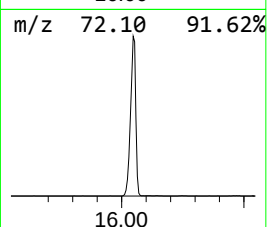
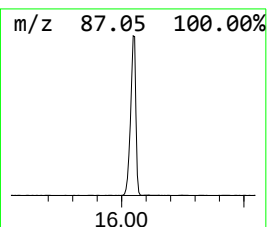
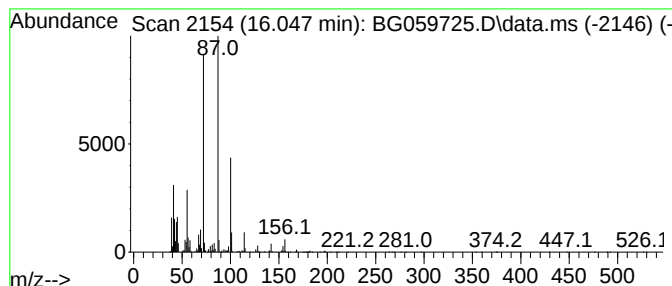
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 N,N-Dimethylheptanamide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.047	413.94 ng	8312980	Acenaphthene-d10	14.966

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N,N-Dimethylheptanamide	157	C9H19NO	001115-96-4	56
2			N,N-Dimethylacetamide	87	C4H9NO	000127-19-5	53
3			Ethanamine, N-ethyl-N-methyl-	87	C5H13N	000616-39-7	50
4			4-Methylheptanamide, N,N-dimethyl-	171	C10H21NO	1000139-77-1	47
5			Isooctanamide, N,N-dimethyl-	171	C10H21NO	1000139-76-9	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111623\
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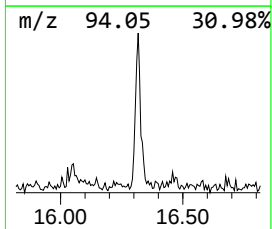
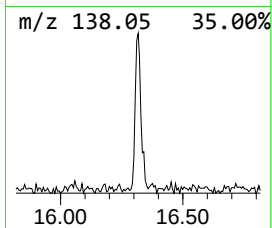
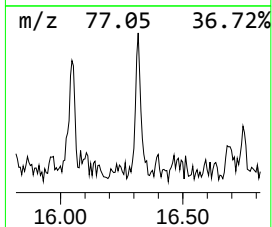
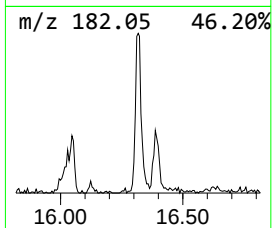
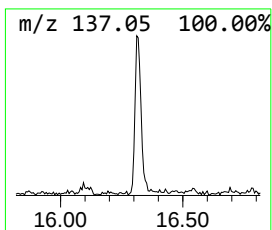
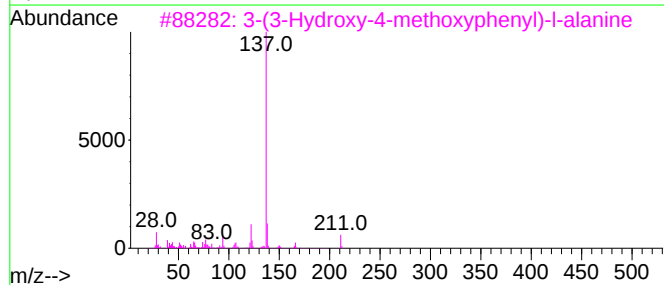
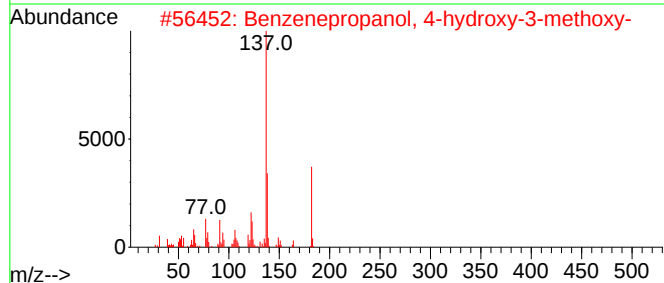
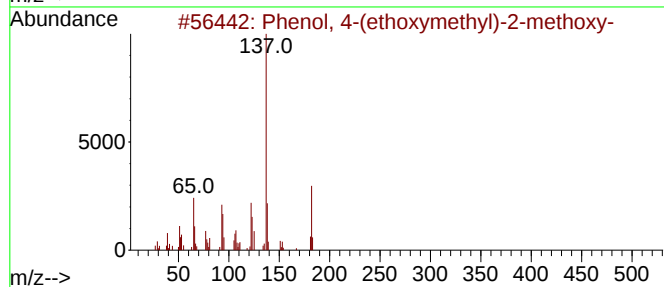
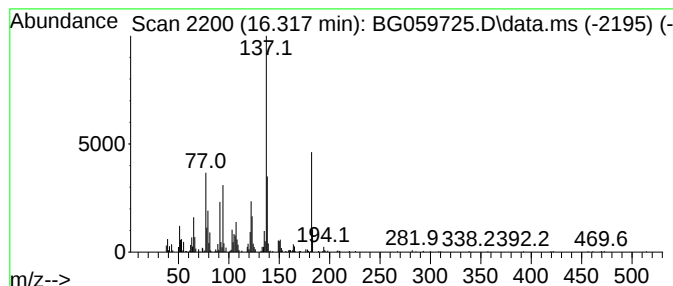
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ClientSampleId :
RD-SW-01-20231103

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Phenol, 4-(ethoxymethyl)-2-... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.317	29.40 ng	590509	Acenaphthene-d10		14.966	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Phenol, 4-(ethoxymethyl)-2-methoxy-		182	C10H14O3	013184-86-6	87
2	Benzenepropanol, 4-hydroxy-3-met...		182	C10H14O3	002305-13-7	83
3	3-(3-Hydroxy-4-methoxyphenyl)-l-...		211	C10H13NO4	1000103-80-4	50
4	Homovanillic acid		182	C9H10O4	000306-08-1	50
5	Ethyl 3,4-dihydroxybenzoate		182	C9H10O4	003943-89-3	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111623\
Data File : BG059725.D
Acq On : 16 Nov 2023 19:36
Operator : MA/JU
Sample : 05415-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RD-SW-01-20231103

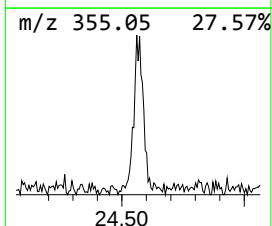
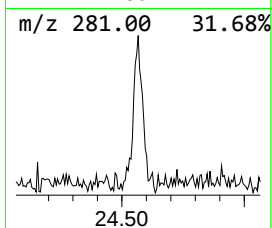
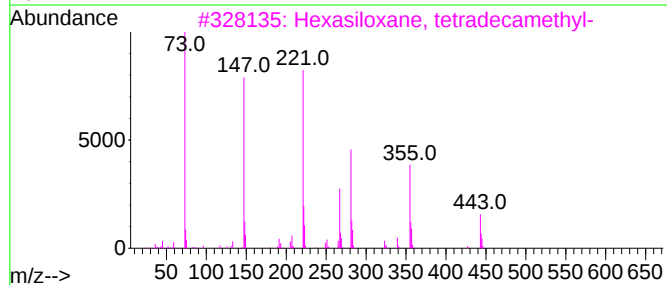
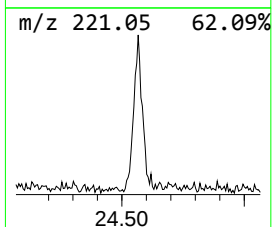
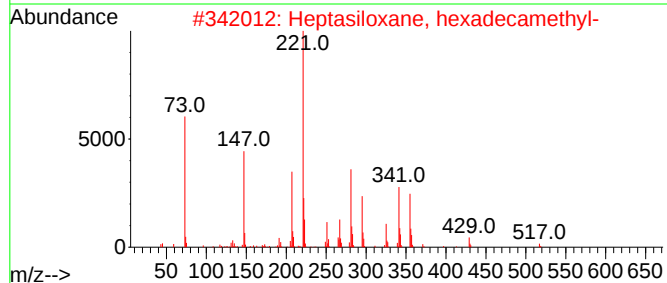
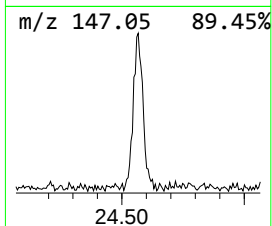
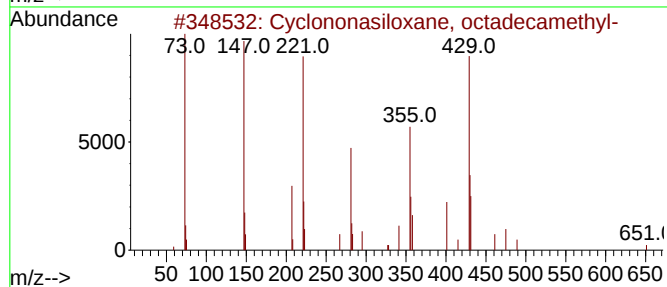
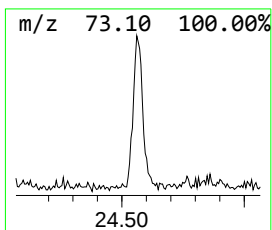
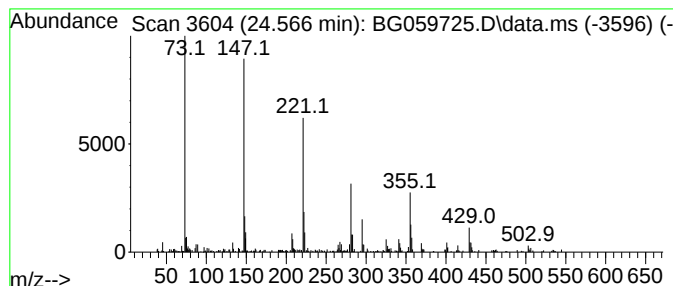
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Cyclononasiloxane, octadeca... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.566	27.64 ng	838907	Perylene-d12	25.636

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	87
2		Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	72
3		Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	64
4		Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	43
5		N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111623\
Data File : BG059725.D
Acq On : 16 Nov 2023 19:36
Operator : MA/JU
Sample : 05415-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RD-SW-01-20231103

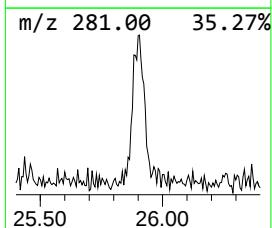
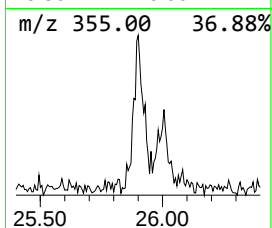
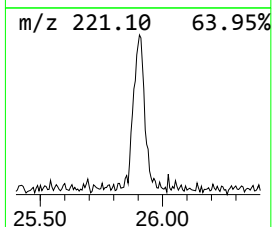
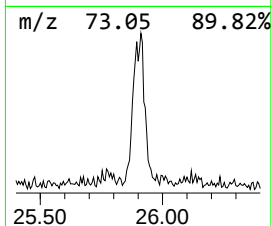
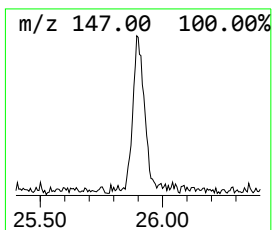
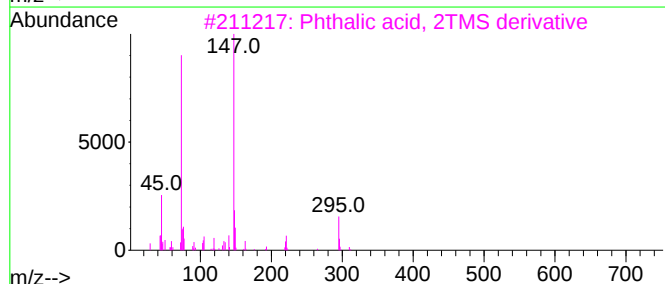
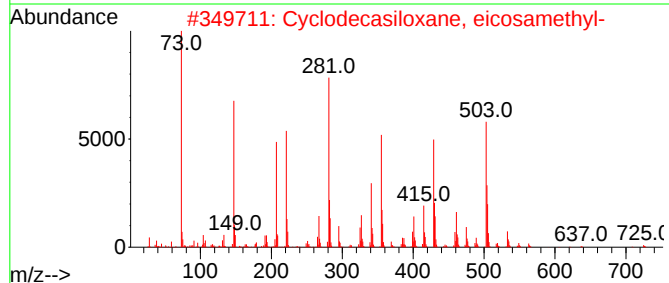
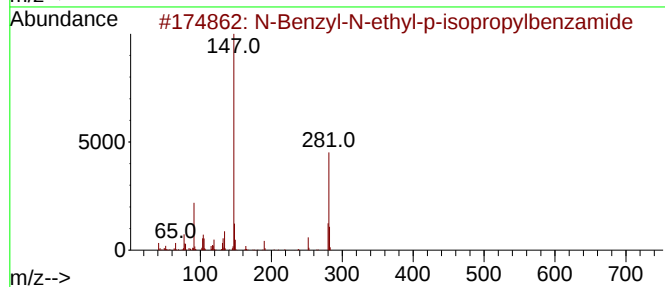
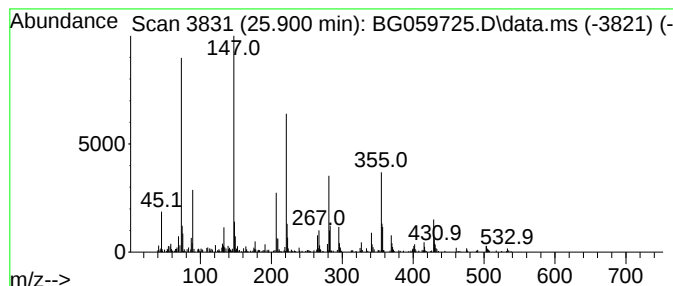
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown25.900 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.900	32.78 ng	994921	Perylene-d12	25.636

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	43
2			Cyclodecasiloxane, eicosamethyl-	740	C20H60O10Si10	018772-36-6	38
3			Phthalic acid, 2TMS derivative	310	C14H22O4Si2	002078-22-0	35
4			(Thiophen-2-ylformamido)olate, 2...	287	C11H21N02SSi2	1000485-22-1	30
5			1,3-Dimethyl-5-pentamethyldisily...	258	C13H30OSi2	1000216-94-7	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111623\
Data File : BG059725.D
Acq On : 16 Nov 2023 19:36
Operator : MA/JU
Sample : 05415-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RD-SW-01-20231103

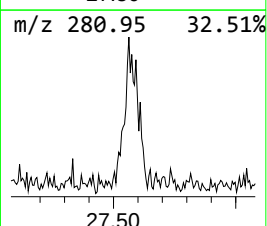
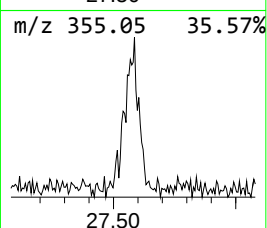
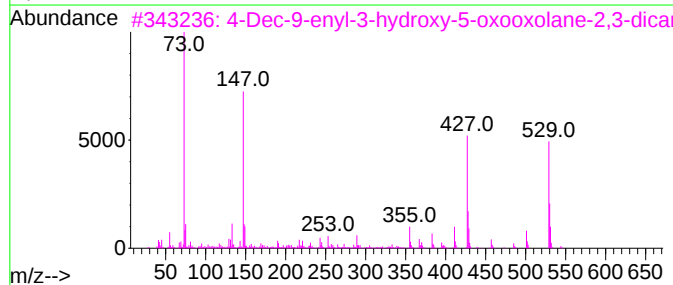
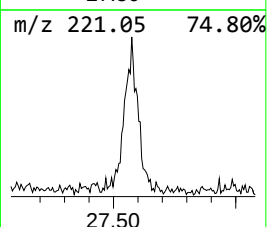
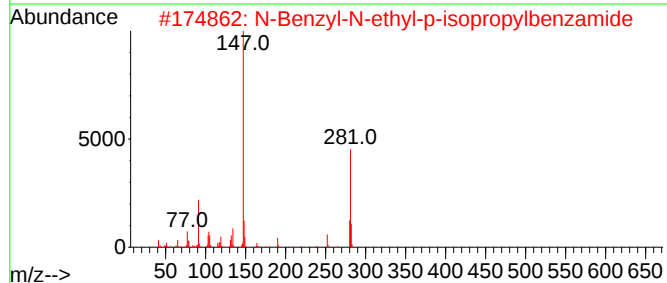
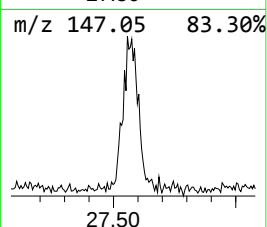
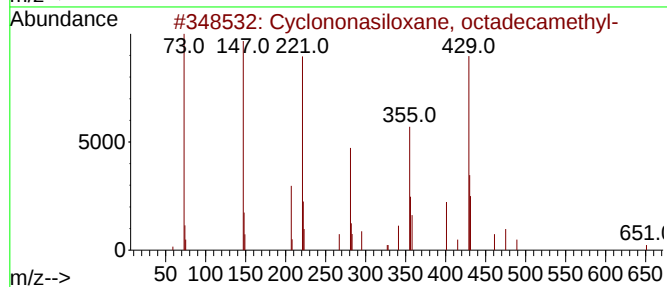
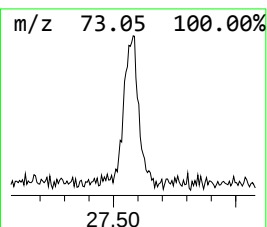
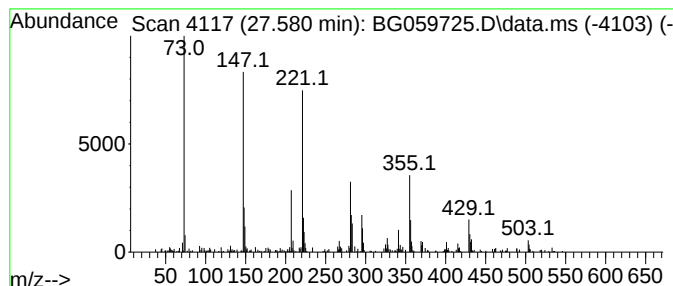
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown27.580 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.580	28.49 ng	864627	Perylene-d12	25.636

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	80
2			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	27
3			4-Dec-9-enyl-3-hydroxy-5-oxooxol...	544	C25H48O7Si3	1000506-08-8	27
4			Bis(4-tert-butyltrimethylsiloxy)b...	458	C26H42O3Si2	1000431-17-0	25
5			1H-Naphtho[2,1-b]pyran-2-carboni...	388	C23H20N2O4	299198-80-4	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111623\
Data File : BG059725.D
Acq On : 16 Nov 2023 19:36
Operator : MA/JU
Sample : 05415-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RD-SW-01-20231103

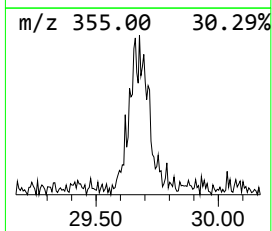
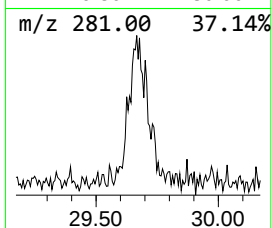
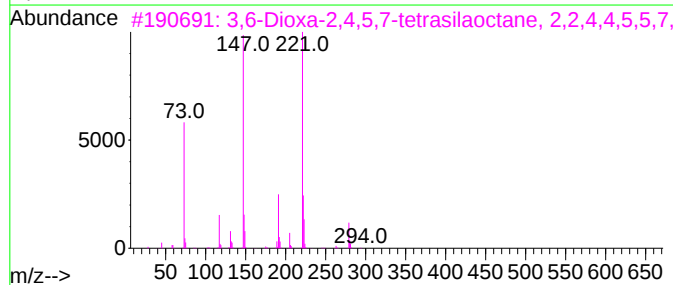
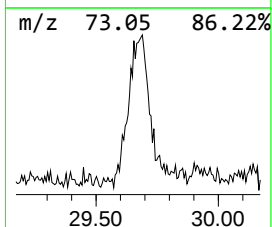
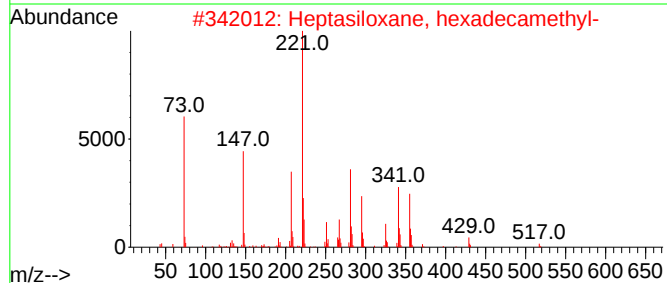
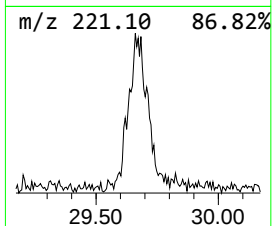
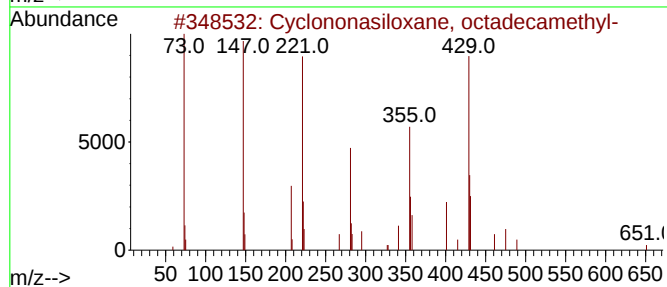
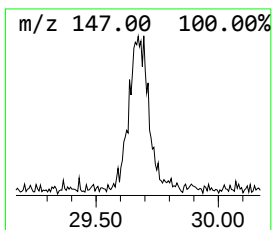
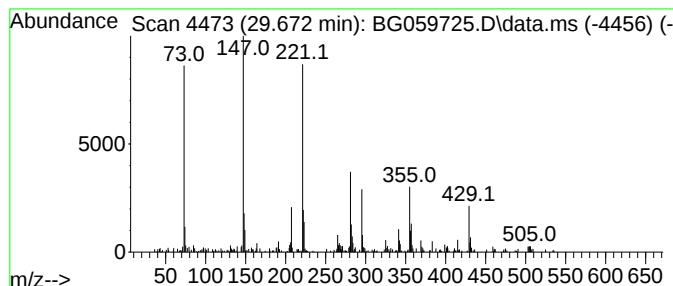
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 unknown29.672 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.672	37.17 ng	1128180	Perylene-d12	25.636

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	59
2		Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	47
3		3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	40
4		4-Hydroxybenzyl alcohol, 2TBDS ...	352	C19H36O2Si2	1000364-43-9	25
5		Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111623\
 Data File : BG059725.D
 Acq On : 16 Nov 2023 19:36
 Operator : MA/JU
 Sample : 05415-03
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RD-SW-01-20231103

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.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
1-Methoxy-1-but...	5.318	28.1	ng	411189	1	8.344	293140	20.0
2-Furanmethanol	5.530	104.2	ng	1527160	1	8.344	293140	20.0
unknown6.517	6.517	31.6	ng	463070	1	8.344	293140	20.0
2-Cyclopenten-1...	8.614	35.1	ng	514849	1	8.344	293140	20.0
Cyclohexane, (1...	9.455	156.3	ng	2290540	1	8.344	293140	20.0
2-Methoxy-5-met...	11.070	118.4	ng	1887340	2	11.188	318833	20.0
unknown11.493	11.493	24.8	ng	394598	2	11.188	318833	20.0
Phenol, 4-ethyl...	12.310	63.0	ng	1003990	2	11.188	318833	20.0
Benzenebutaneni...	13.174	98.9	ng	1985810	3	14.966	401655	20.0
Phenol, 2,6-dim...	13.244	102.8	ng	2064440	3	14.966	401655	20.0
unknown14.302	14.302	57.5	ng	1154690	3	14.966	401655	20.0
Apocynin	14.819	35.3	ng	709134	3	14.966	401655	20.0
4-Ethyl-2,6-dim...	15.083	31.6	ng	635557	3	14.966	401655	20.0
2-Propanone, 1-...	15.213	48.9	ng	980999	3	14.966	401655	20.0
N,N-Dimethylhep...	16.047	413.9	ng	8312980	3	14.966	401655	20.0
Phenol, 4-(etho...	16.317	29.4	ng	590509	3	14.966	401655	20.0
Cyclononasiloxa...	24.566	27.6	ng	838907	6	25.636	606975	20.0
unknown25.900	25.900	32.8	ng	994921	6	25.636	606975	20.0
unknown27.580	27.580	28.5	ng	864627	6	25.636	606975	20.0
unknown29.672	29.672	37.2	ng	1128180	6	25.636	606975	20.0