

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
 Data File : BF128056.D
 Acq On : 03 May 2022 20:09
 Operator : CG\JU
 Sample : N2659-04
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 22L097-D

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-BF042222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128056.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.528	377	381	387	rVB	157463	165481	3.51%	0.363%
2	5.169	480	490	493	rBV	2429874	4715265	100.00%	10.334%
3	5.534	549	552	560	rVB	130633	122342	2.59%	0.268%
4	5.857	603	607	619	rBV	69129	68963	1.46%	0.151%
5	6.175	653	661	664	rBV	603748	818053	17.35%	1.793%
6	6.422	697	703	709	rBV2	51875	90062	1.91%	0.197%
7	6.540	719	723	731	rVB	1132349	1091405	23.15%	2.392%
8	6.916	783	787	790	rBV	705369	579431	12.29%	1.270%
9	6.969	792	796	803	rBV	42893	51378	1.09%	0.113%
10	7.481	878	883	886	rBV	1686269	1549762	32.87%	3.397%
11	8.104	983	989	997	rBV	1951185	2266923	48.08%	4.968%
12	8.169	997	1000	1002	rVV	89609	90917	1.93%	0.199%
13	8.198	1002	1005	1007	rVV	926918	747125	15.84%	1.637%
14	8.222	1007	1009	1011	rVV	277100	220443	4.68%	0.483%
15	8.775	1098	1103	1107	rBV2	108491	98450	2.09%	0.216%
16	8.910	1123	1126	1129	rVB	222224	166007	3.52%	0.364%
17	9.010	1138	1143	1146	rBV	129137	105020	2.23%	0.230%
18	9.275	1183	1188	1191	rBV	3126569	2536993	53.80%	5.560%
19	9.345	1196	1200	1202	rBV	141071	129401	2.74%	0.284%
20	9.380	1202	1206	1211	rVB2	252291	234075	4.96%	0.513%
21	9.533	1229	1232	1237	rBV	48229	66321	1.41%	0.145%
22	9.610	1241	1245	1248	rVV2	61972	71817	1.52%	0.157%
23	9.663	1251	1254	1256	rVB	55930	51967	1.10%	0.114%
24	9.875	1286	1290	1294	rVB	172706	138996	2.95%	0.305%
25	9.957	1294	1304	1307	rBV	930900	804709	17.07%	1.764%
26	9.986	1307	1309	1312	rVB	124905	111228	2.36%	0.244%
27	10.098	1325	1328	1332	rVV4	46102	58567	1.24%	0.128%
28	10.163	1335	1339	1342	rVV2	121732	121386	2.57%	0.266%
29	10.192	1342	1344	1349	rVB2	47397	48443	1.03%	0.106%
30	10.351	1368	1371	1373	rBV	50140	62400	1.32%	0.137%
31	10.375	1373	1375	1378	rVV	151693	113485	2.41%	0.249%
32	10.404	1378	1380	1383	rVV	110856	89503	1.90%	0.196%
33	10.504	1394	1397	1400	rBV2	193788	162910	3.45%	0.357%
34	10.533	1400	1402	1404	rVV2	60136	61069	1.30%	0.134%
35	10.557	1404	1406	1409	rVB	73062	58409	1.24%	0.128%
36	10.592	1409	1412	1414	rBV2	74554	72266	1.53%	0.158%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
 Data File : BF128056.D
 Acq On : 03 May 2022 20:09
 Operator : CG\JU
 Sample : N2659-04
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 22L097-D

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-BF042222.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	10.622	1415	1417	1419	rVV	73054	63701	1.35%	0.140%
38	10.663	1421	1424	1428	rVV2	173584	179083	3.80%	0.392%
39	10.704	1428	1431	1433	rVV	328567	342166	7.26%	0.750%
40	10.722	1433	1434	1436	rVV	243184	155013	3.29%	0.340%
41	10.745	1436	1438	1443	rVB2	224314	228999	4.86%	0.502%
42	10.816	1448	1450	1454	rVV3	37921	54738	1.16%	0.120%
43	10.875	1454	1460	1462	rVV	884724	960953	20.38%	2.106%
44	10.927	1465	1469	1471	rVV	2261770	2117696	44.91%	4.641%
45	10.963	1471	1475	1478	rVV2	2408017	3062332	64.95%	6.712%
46	10.992	1478	1480	1483	rVV2	2341731	2275939	48.27%	4.988%
47	11.016	1483	1484	1487	rVV	1281609	1084316	23.00%	2.376%
48	11.045	1487	1489	1491	rVV	866350	971104	20.59%	2.128%
49	11.075	1493	1494	1496	rVV	777495	481479	10.21%	1.055%
50	11.104	1496	1499	1503	rVV3	1552175	1910641	40.52%	4.188%
51	11.145	1503	1506	1508	rVV	2172164	2042402	43.31%	4.476%
52	11.186	1511	1513	1522	rVV2	1071904	1031034	21.87%	2.260%
53	11.263	1522	1526	1529	rVV	149713	179649	3.81%	0.394%
54	11.298	1529	1532	1534	rVV2	158811	168290	3.57%	0.369%
55	11.327	1534	1537	1539	rVV	246344	268097	5.69%	0.588%
56	11.351	1539	1541	1543	rVV2	118996	120275	2.55%	0.264%
57	11.374	1543	1545	1546	rVV2	111127	92732	1.97%	0.203%
58	11.398	1546	1549	1553	rVV	714804	613644	13.01%	1.345%
59	11.451	1553	1558	1560	rVV	737454	662139	14.04%	1.451%
60	11.474	1560	1562	1568	rVV	777710	641784	13.61%	1.407%
61	11.527	1568	1571	1573	rVV	160860	137099	2.91%	0.300%
62	11.551	1573	1575	1579	rVB2	411966	326567	6.93%	0.716%
63	11.616	1583	1586	1590	rBV5	48562	60935	1.29%	0.134%
64	11.657	1590	1593	1595	rVV	143044	123025	2.61%	0.270%
65	11.680	1595	1597	1601	rVB	86665	71320	1.51%	0.156%
66	11.727	1602	1605	1607	rVV	78893	59383	1.26%	0.130%
67	11.951	1639	1643	1646	rBV	104768	117923	2.50%	0.258%
68	11.980	1646	1648	1651	rVV	134130	106770	2.26%	0.234%
69	12.063	1659	1662	1665	rVV	119027	144451	3.06%	0.317%
70	12.133	1671	1674	1676	rBV	87611	68191	1.45%	0.149%
71	12.245	1691	1693	1695	rBV	63958	49451	1.05%	0.108%
72	12.274	1695	1698	1703	rVB3	55326	62055	1.32%	0.136%
73	12.498	1733	1736	1738	rBV	64997	70318	1.49%	0.154%
74	12.521	1738	1740	1745	rVV4	89540	138626	2.94%	0.304%
75	12.592	1749	1752	1755	rBV2	39937	47515	1.01%	0.104%
76	12.669	1761	1765	1768	rBV	711651	615925	13.06%	1.350%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
 Data File : BF128056.D
 Acq On : 03 May 2022 20:09
 Operator : CG\JU
 Sample : N2659-04
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 22L097-D

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-BF042222.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	12.786	1783	1785	1789	rBV3	39652	65624	1.39%	0.144%
78	12.898	1801	1804	1807	rVB	598791	440466	9.34%	0.965%
79	13.039	1821	1828	1831	rBV	2134598	1983973	42.08%	4.348%
80	13.221	1857	1859	1862	rVB	76145	67314	1.43%	0.148%
81	13.251	1862	1864	1867	rBV2	71008	66901	1.42%	0.147%
82	13.292	1868	1871	1873	rVB	66660	55965	1.19%	0.123%
83	13.327	1875	1877	1880	rVB2	60157	50222	1.07%	0.110%
84	13.451	1896	1898	1901	rBV	52384	59395	1.26%	0.130%
85	13.598	1920	1923	1925	rBV	74181	70456	1.49%	0.154%
86	13.927	1977	1979	1990	rVB4	149779	298139	6.32%	0.653%
87	14.010	1991	1993	1996	rBV2	112413	103611	2.20%	0.227%
88	14.068	2000	2003	2005	rBV2	265465	309796	6.57%	0.679%
89	14.098	2005	2008	2011	rVV2	640860	756957	16.05%	1.659%
90	14.121	2011	2012	2017	rVB2	241225	210210	4.46%	0.461%
91	14.204	2024	2026	2028	rBV2	73878	50265	1.07%	0.110%
92	14.245	2030	2033	2035	rVV	83060	83607	1.77%	0.183%
93	14.715	2110	2113	2116	rVB	289148	240078	5.09%	0.526%
94	15.157	2185	2188	2195	rBV	169634	288476	6.12%	0.632%
95	15.539	2250	2253	2259	rVB	132118	166045	3.52%	0.364%
96	15.610	2261	2265	2269	rBV	338647	410747	8.71%	0.900%

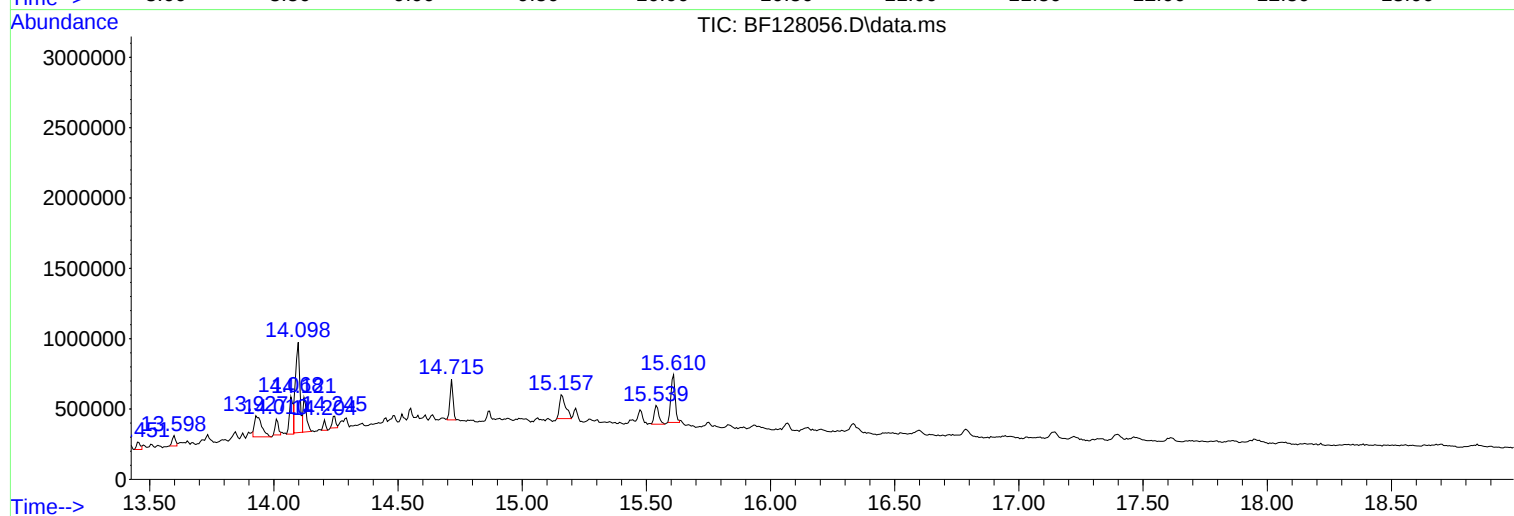
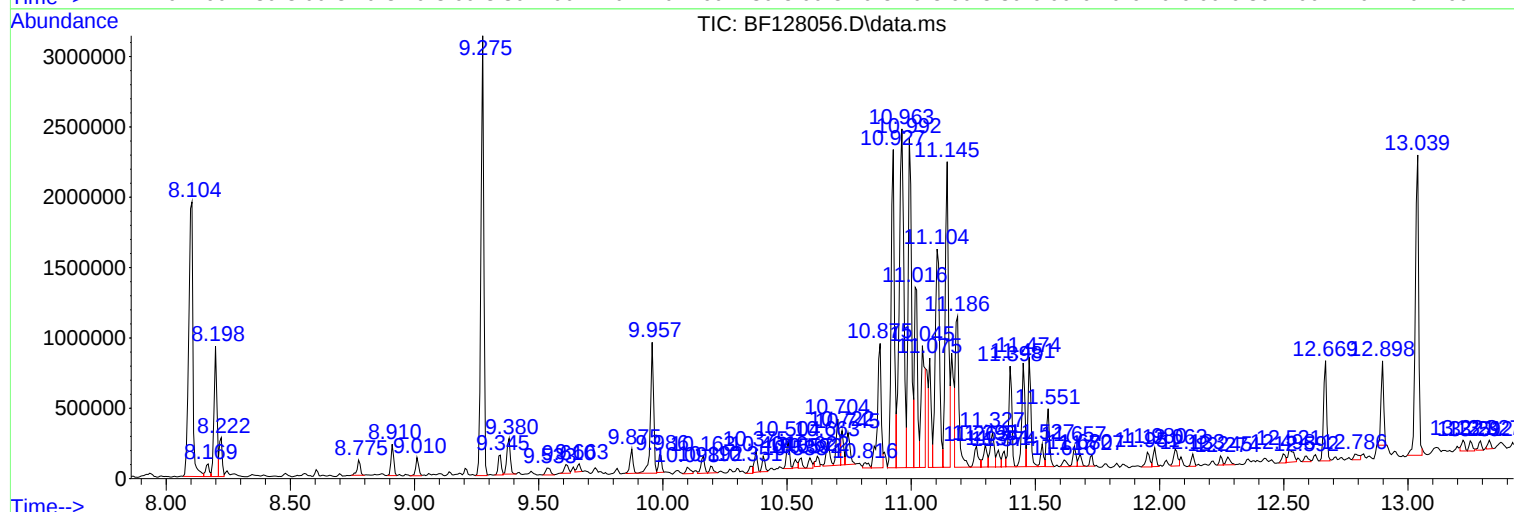
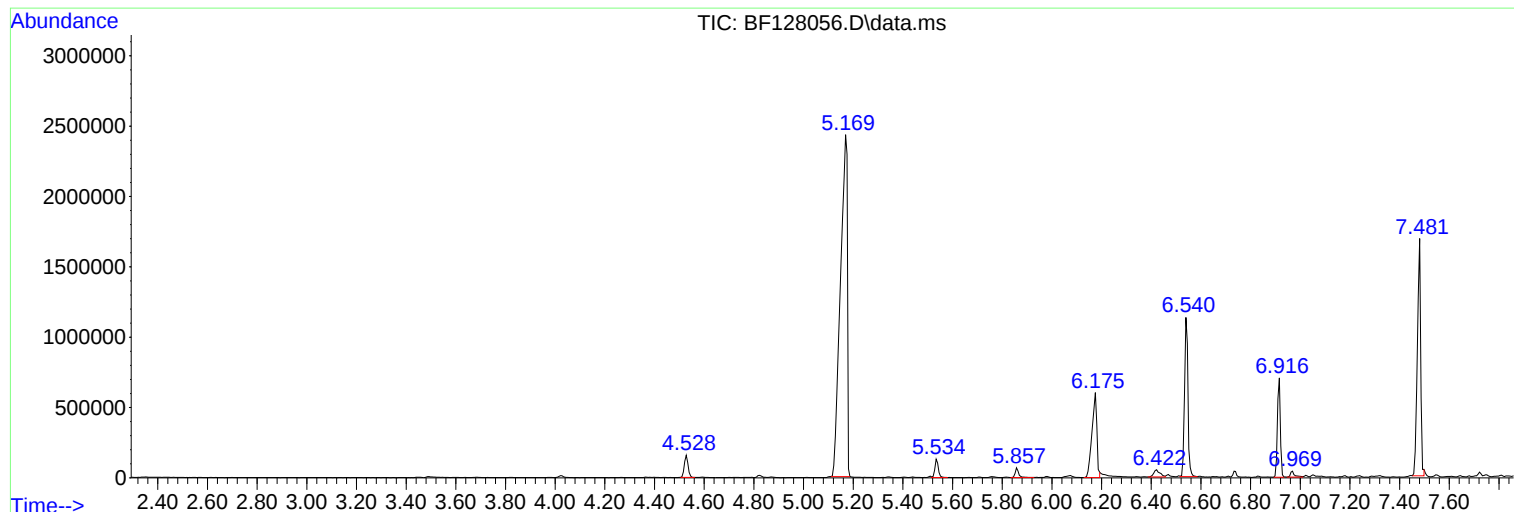
Sum of corrected areas: 45626979

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
Data File : BF128056.D
Acq On : 03 May 2022 20:09
Operator : CG\JU
Sample : N2659-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
Data File : BF128056.D
Acq On : 03 May 2022 20:09
Operator : CG\JU
Sample : N2659-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-D

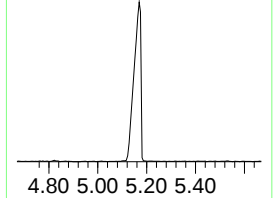
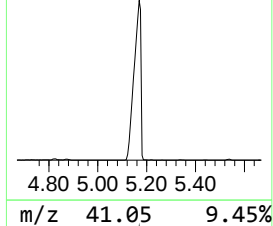
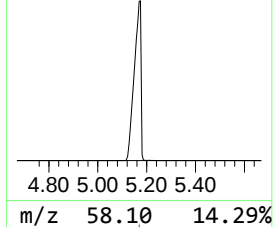
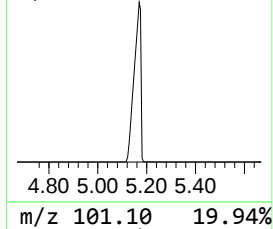
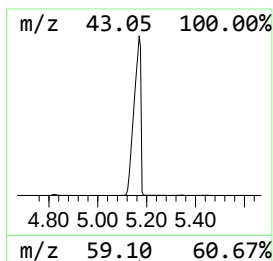
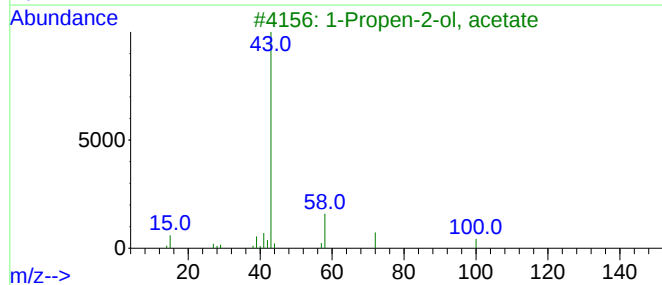
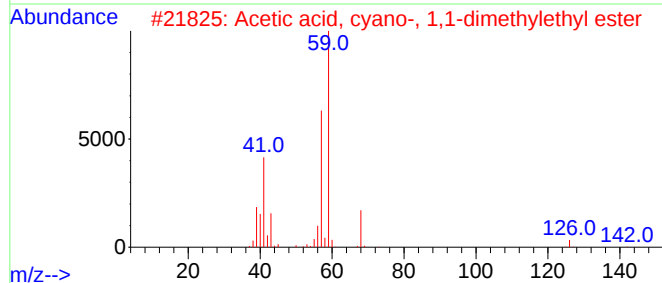
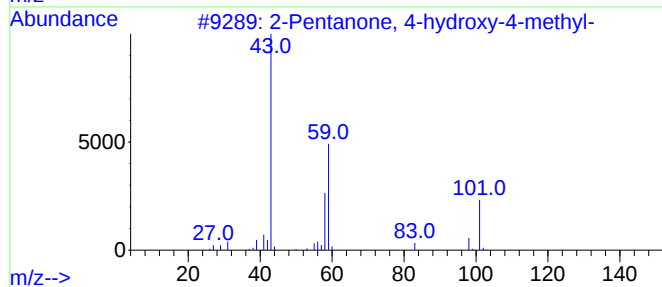
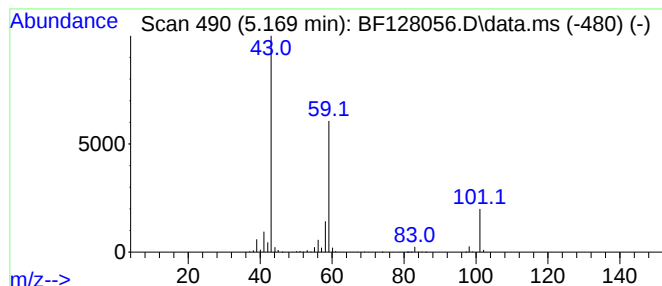
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.169	162.76 ng	4715270	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
Data File : BF128056.D
Acq On : 03 May 2022 20:09
Operator : CG\JU
Sample : N2659-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-D

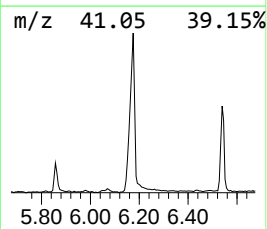
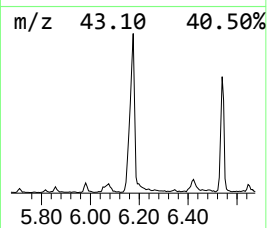
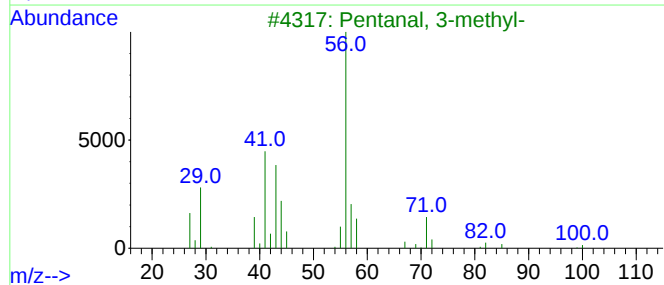
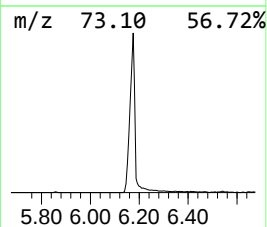
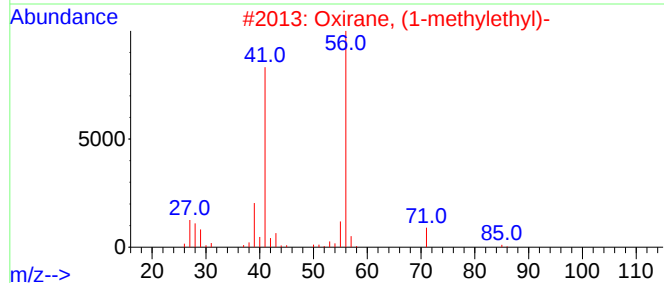
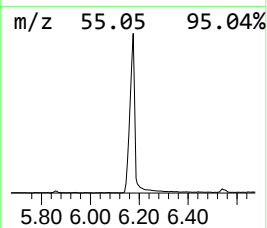
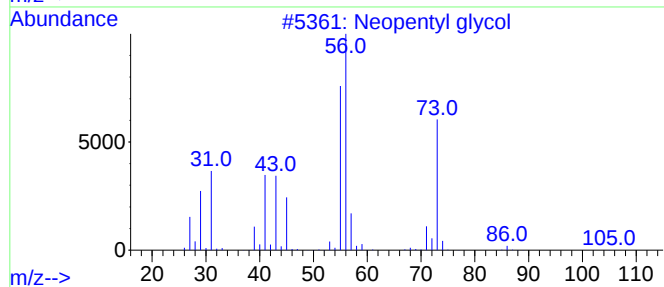
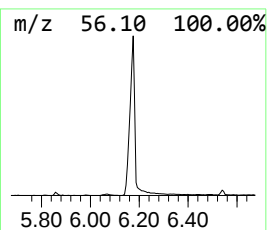
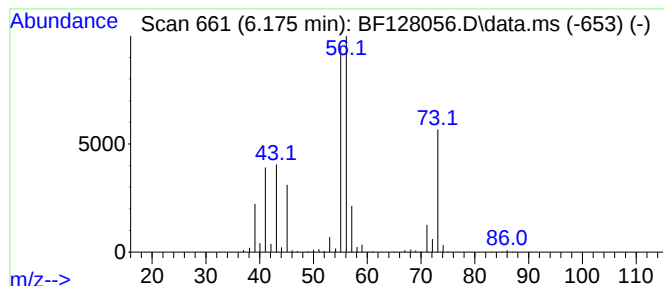
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Neopentyl glycol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.175	28.24 ng	818053	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Neopentyl glycol	104	C5H12O2	000126-30-7	83
2			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	47
3			Pentanal, 3-methyl-	100	C6H12O	015877-57-3	33
4			1-Hepten-4-ol	114	C7H14O	003521-91-3	12
5			4-Heptanol	116	C7H16O	000589-55-9	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
Data File : BF128056.D
Acq On : 03 May 2022 20:09
Operator : CG\JU
Sample : N2659-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-D

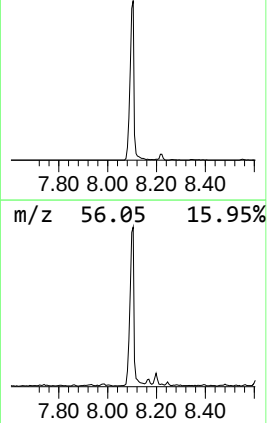
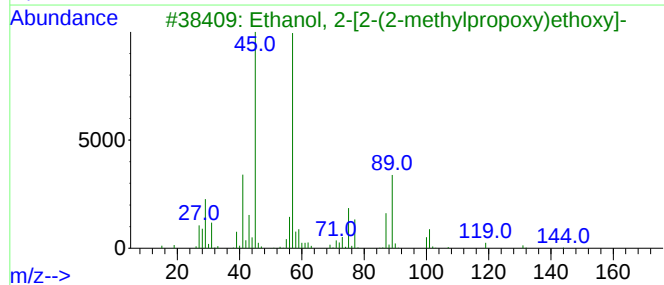
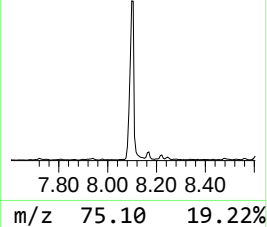
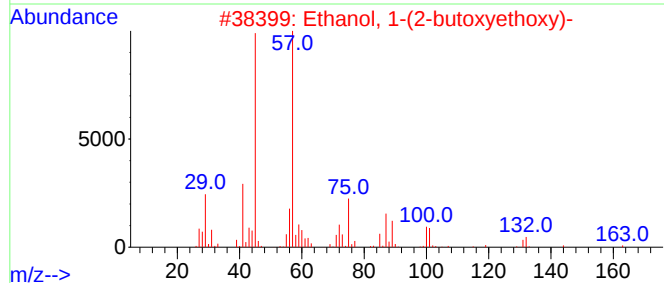
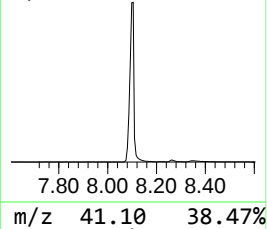
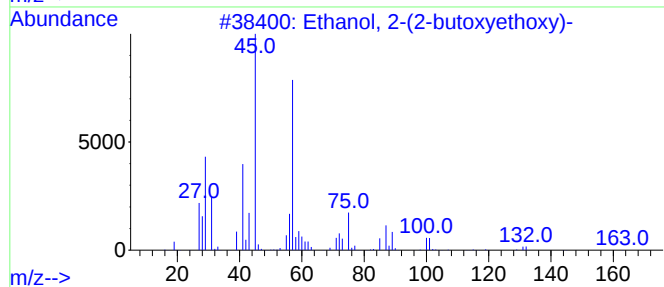
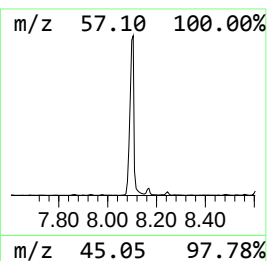
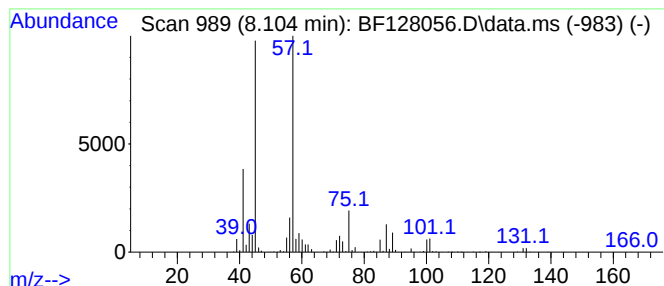
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.104	60.68 ng	2266920	Naphthalene-d8	8.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
Data File : BF128056.D
Acq On : 03 May 2022 20:09
Operator : CG\JU
Sample : N2659-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-D

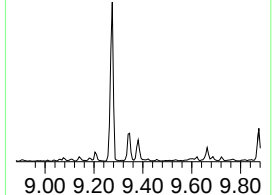
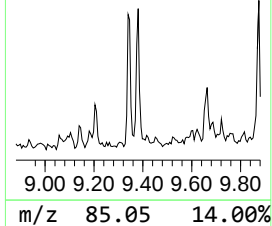
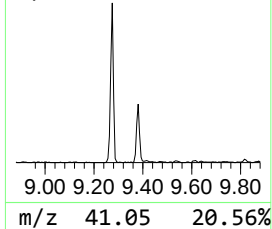
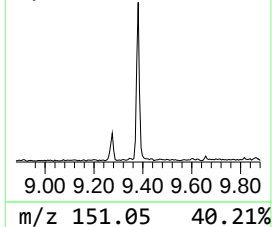
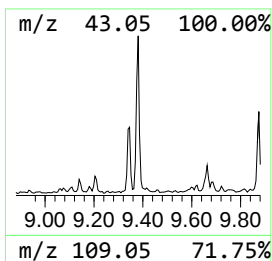
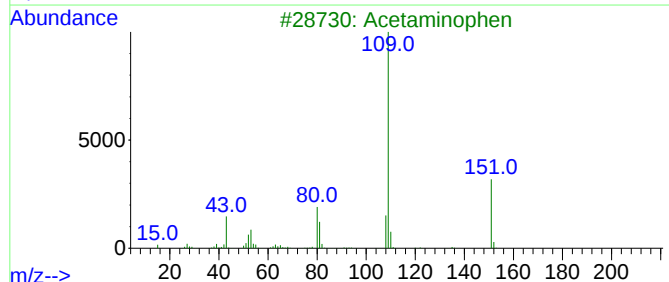
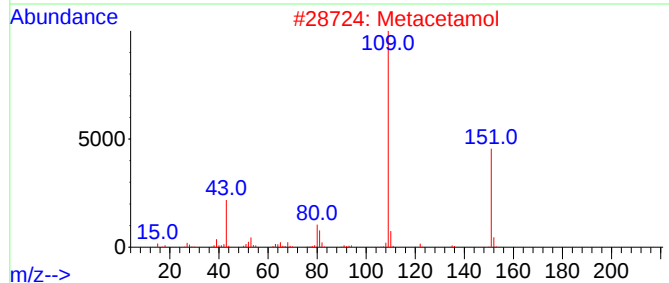
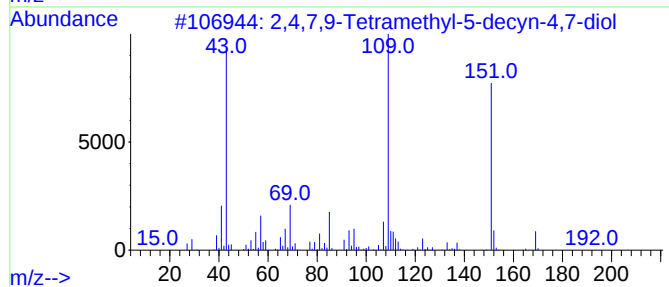
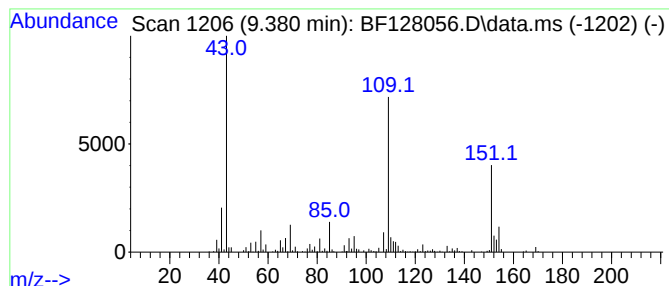
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.380	5.82 ng	234075	Acenaphthene-d10	9.957

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87	
2	Metacetamol	151	C8H9NO2	000621-42-1	47	
3	Acetaminophen	151	C8H9NO2	000103-90-2	47	
4	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	40	
5	(4-Fluorophenyl) methanol, ethyl...	154	C9H11FO	1000374-63-4	35	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
Data File : BF128056.D
Acq On : 03 May 2022 20:09
Operator : CG\JU
Sample : N2659-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-D

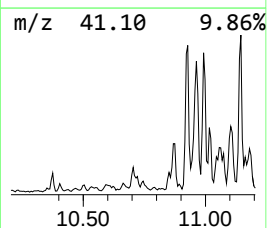
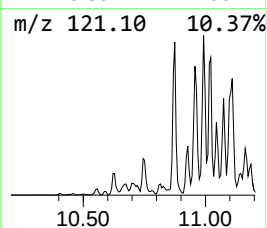
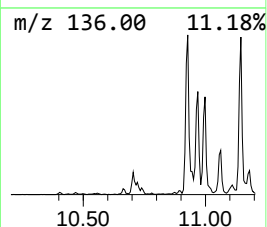
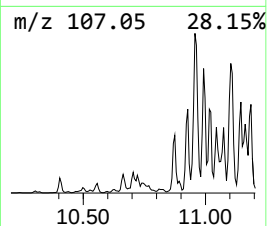
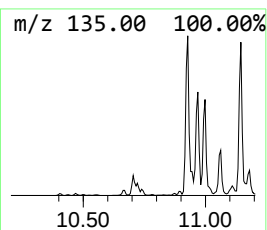
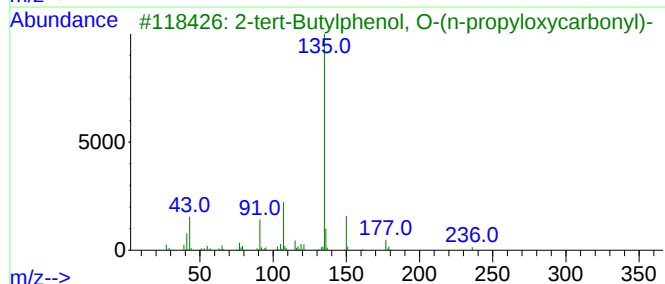
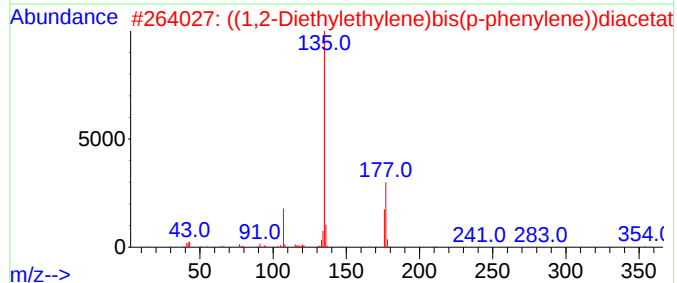
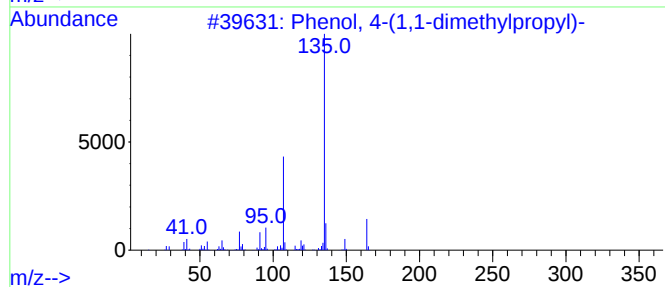
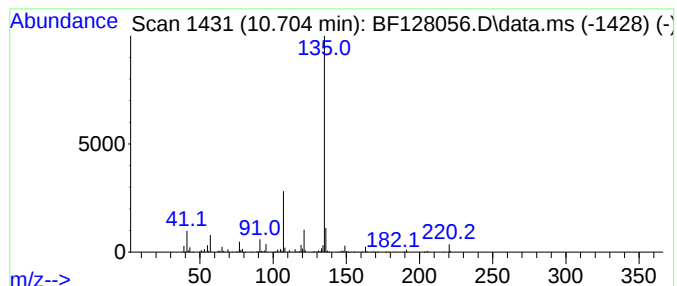
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Phenol, 4-(1,1-dimethylprop... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.704	10.34 ng	342166	Phenanthrene-d10	11.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	87
2			((1,2-Diethylethylene)bis(p-phen...	354	C22H26O4	004547-76-6	64
3			2-tert-Butylphenol, O-(n-propylo...	236	C14H20O3	1000487-37-9	64
4			Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	64
5			Hexestrol, O-trifluoroacetyl-	366	C20H21F3O3	1000365-31-7	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
Data File : BF128056.D
Acq On : 03 May 2022 20:09
Operator : CG\JU
Sample : N2659-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-D

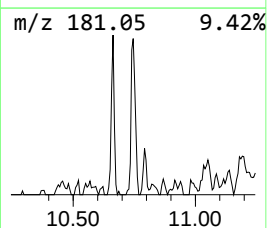
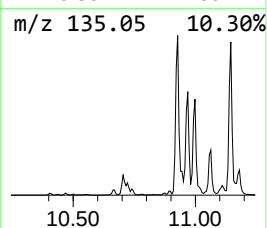
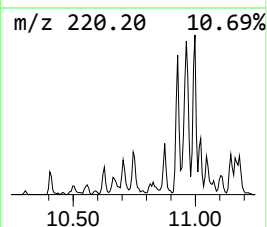
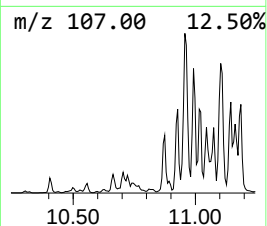
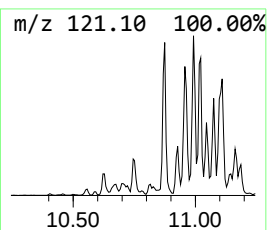
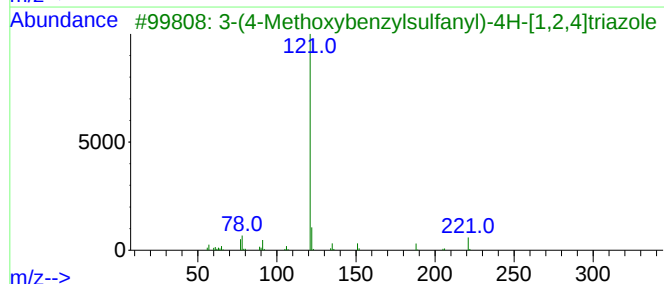
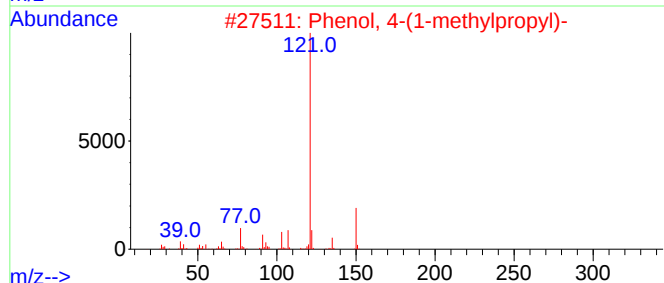
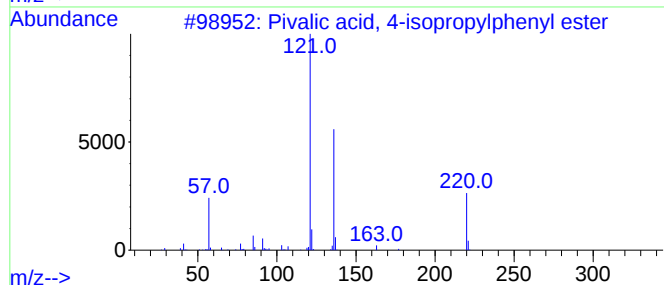
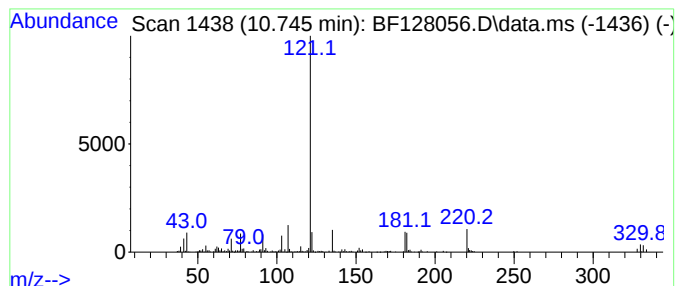
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pivalic acid, 4-isopropylph... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.745	6.92 ng	228999	Phenanthrene-d10	11.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pivalic acid, 4-isopropylphenyl ...	220	C14H20O2	1000330-92-0	53
2			Phenol, 4-(1-methylpropyl)-	150	C10H14O	000099-71-8	53
3			3-(4-Methoxybenzylsulfanyl)-4H-[...]	221	C10H11N3OS	1000306-37-8	50
4			4-(2,4-Dimethyl-phenylcarbamoyl)...	235	C13H17NO3	1000317-38-5	50
5			2-(4-Methoxyphenyl)ethanol	152	C9H12O2	000702-23-8	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
Data File : BF128056.D
Acq On : 03 May 2022 20:09
Operator : CG\JU
Sample : N2659-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-D

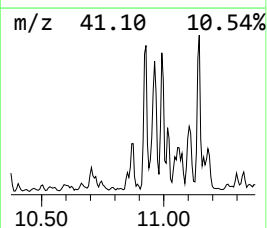
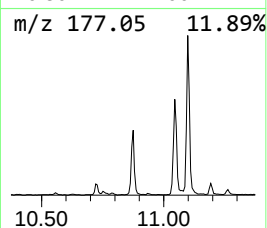
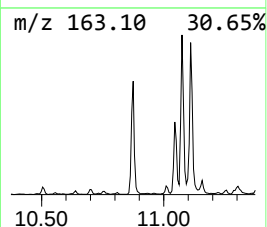
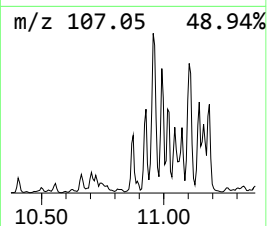
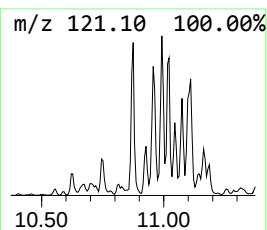
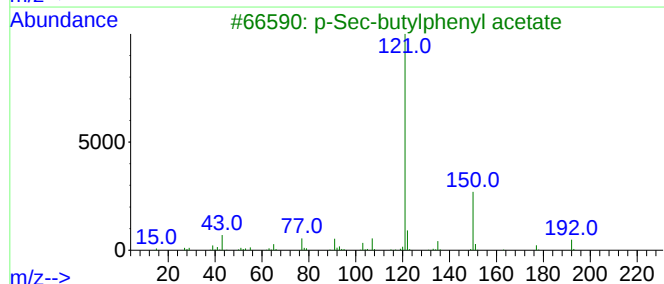
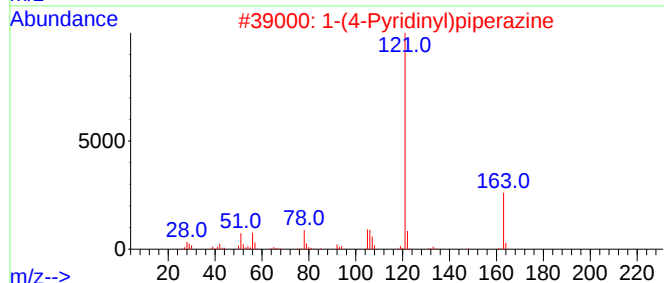
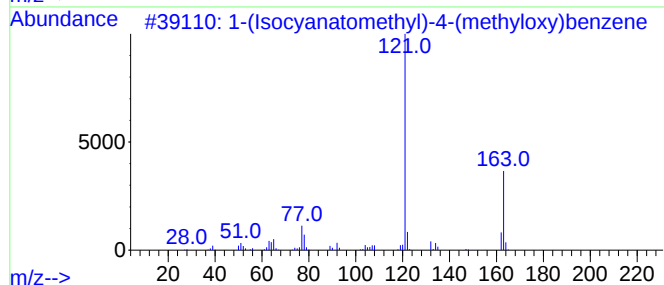
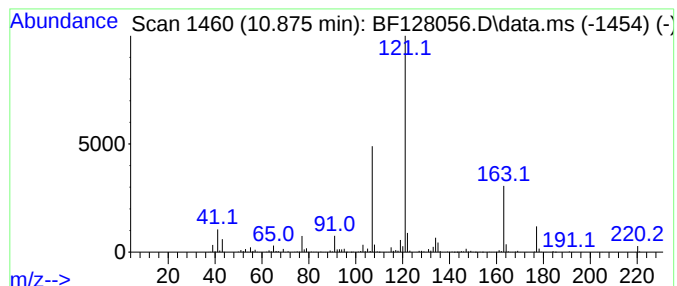
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-(Isocyanatomethyl)-4-(met... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.874	29.03 ng	960953	Phenanthrene-d10	11.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(Isocyanatomethyl)-4-(methylox...	163	C9H9NO2	056651-60-6	53		
2	1-(4-Pyridinyl)piperazine	163	C9H13N3	001008-91-9	50		
3	p-Sec-butylphenyl acetate	192	C12H16O2	003245-24-7	43		
4	2-Propanone, 1-(4-methoxyphenyl)-	164	C10H12O2	000122-84-9	43		
5	Carbonic acid, isobutyl 4-isopro...	236	C14H20O3	1000331-40-6	38		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
Data File : BF128056.D
Acq On : 03 May 2022 20:09
Operator : CG\JU
Sample : N2659-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

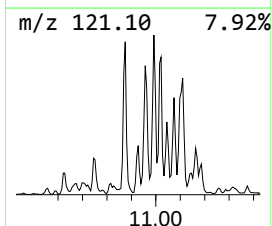
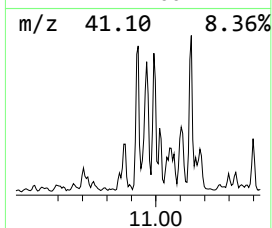
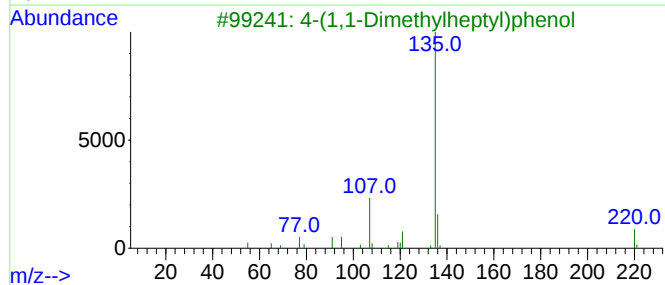
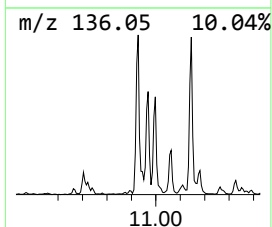
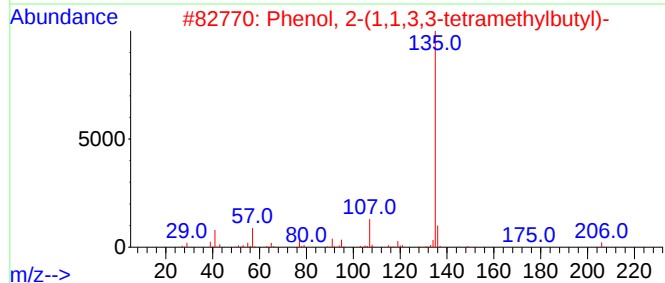
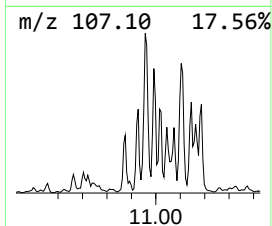
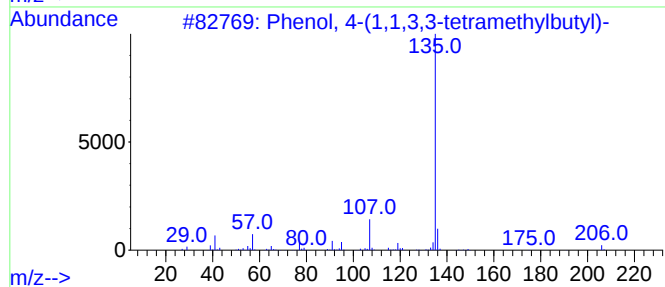
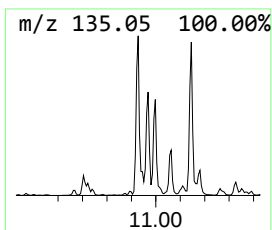
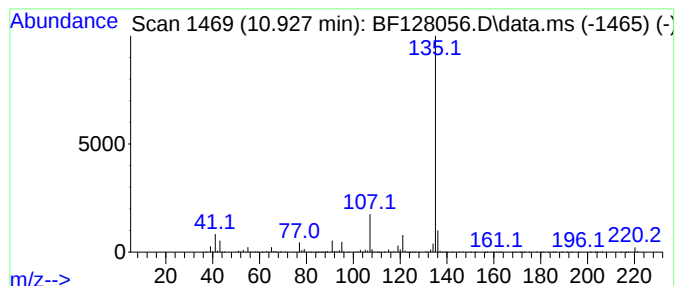
Instrument :
BNA_F
ClientSampleId :
22L097-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
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-(1,1,3,3-tetramet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.928	63.97 ng	2117700	Phenanthrene-d10	11.451	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	90
2	Phenol, 2-(1,1,3,3-tetramethylbu...	206	C14H22O	003884-95-5	90
3	4-(1,1-Dimethylheptyl)phenol	220	C15H24O	1000384-80-3	80
4	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	78
5	4-tert-Butylphenyl acetate	192	C12H16O2	003056-64-2	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
Data File : BF128056.D
Acq On : 03 May 2022 20:09
Operator : CG\JU
Sample : N2659-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

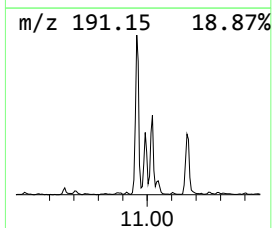
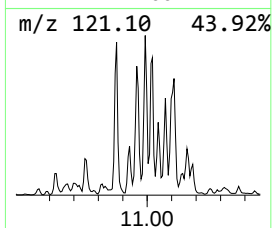
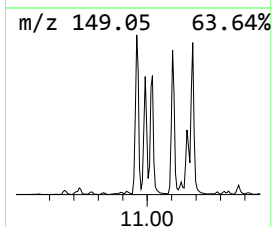
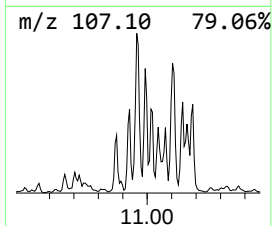
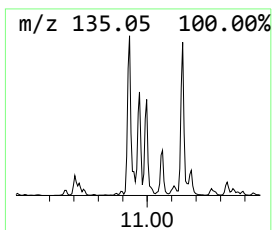
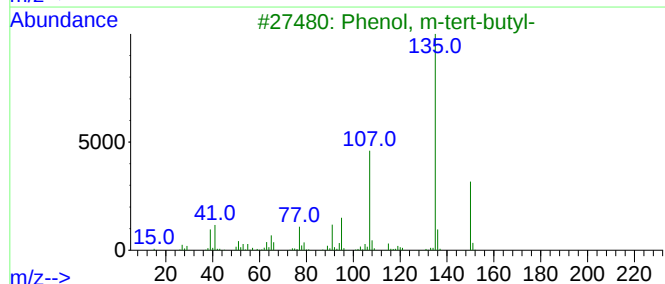
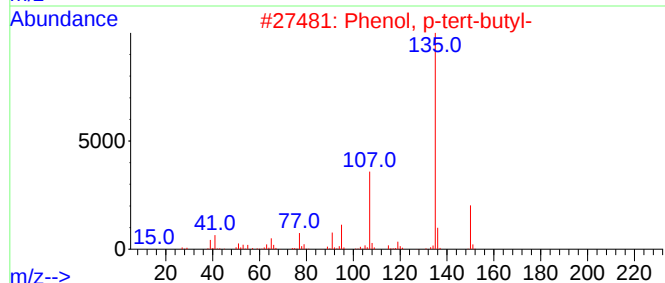
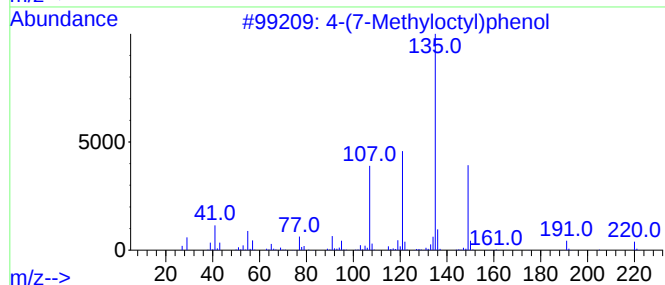
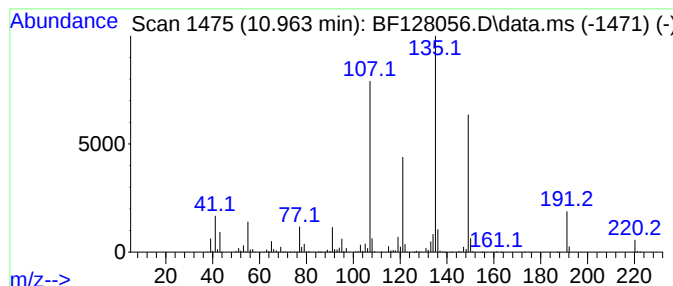
Instrument :
BNA_F
ClientSampleId :
22L097-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 4-(7-Methyloctyl)phenol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.963	92.50 ng	3062330	Phenanthrene-d10	11.451	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(7-Methyloctyl)phenol	220	C15H24O	024518-48-7	91
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	58
3	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	58
4	1-(Isocyanatomethyl)-4-propoxybe...	191	C11H13NO2	936095-07-7	38
5	1H-Indole, 5-fluoro-	135	C8H6FN	000399-52-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
Data File : BF128056.D
Acq On : 03 May 2022 20:09
Operator : CG\JU
Sample : N2659-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-D

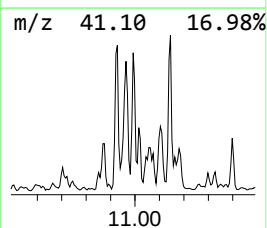
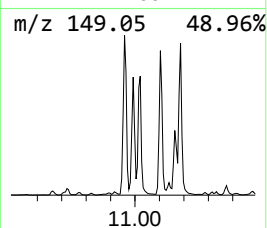
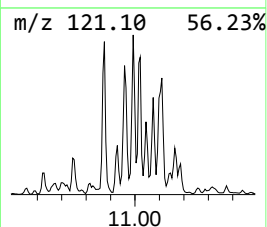
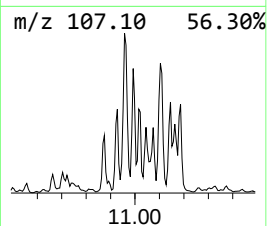
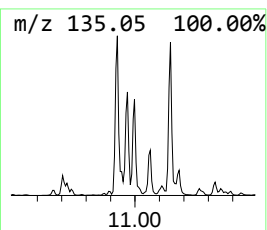
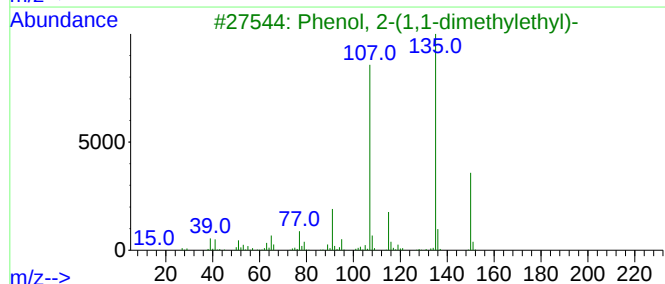
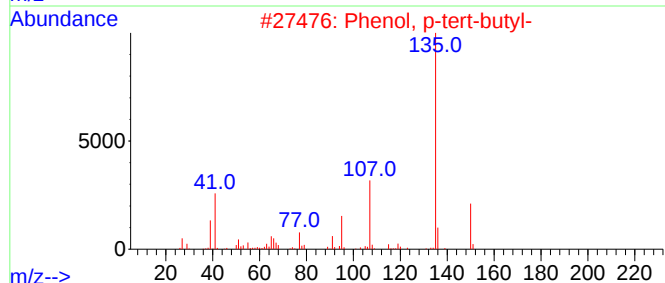
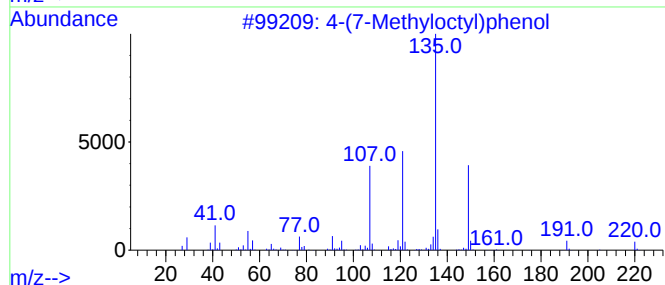
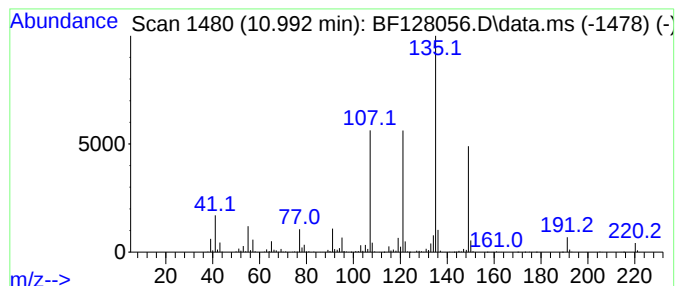
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Phenol, p-tert-butyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.992	68.75 ng	2275940	Phenanthrene-d10	11.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(7-Methyloctyl)phenol			220	C15H24O	024518-48-7	98
2	Phenol, p-tert-butyl-			150	C10H14O	000098-54-4	58
3	Phenol, 2-(1,1-dimethylethyl)-			150	C10H14O	000088-18-6	52
4	Phenol, 4-(1,1-dimethylpropyl)-			164	C11H16O	000080-46-6	50
5	((1,2-Diethylethylene)bis(p-phen...			354	C22H26O4	004547-76-6	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
Data File : BF128056.D
Acq On : 03 May 2022 20:09
Operator : CG\JU
Sample : N2659-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-D

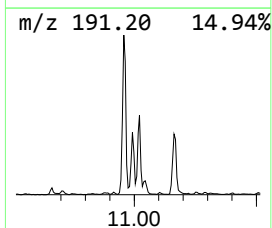
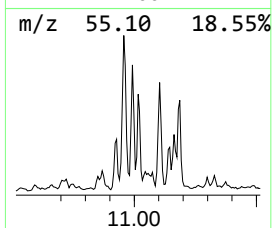
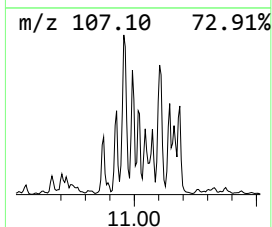
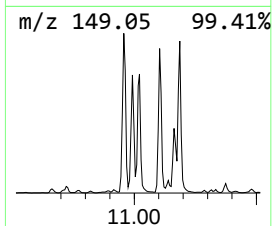
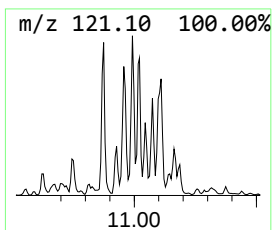
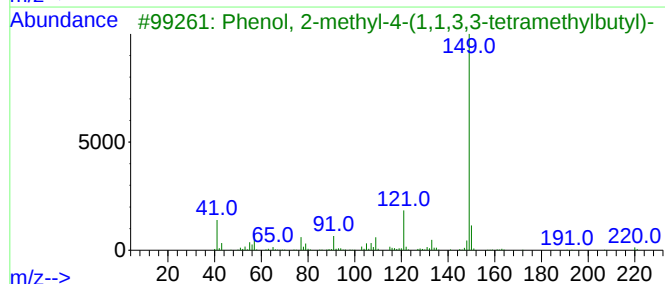
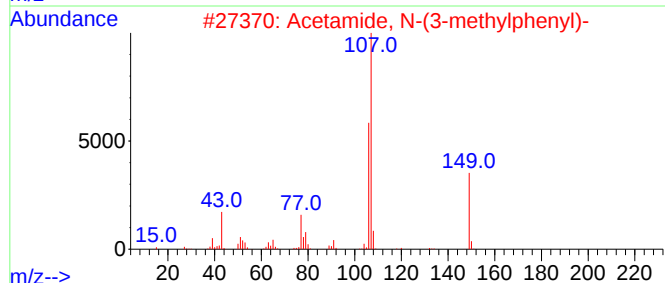
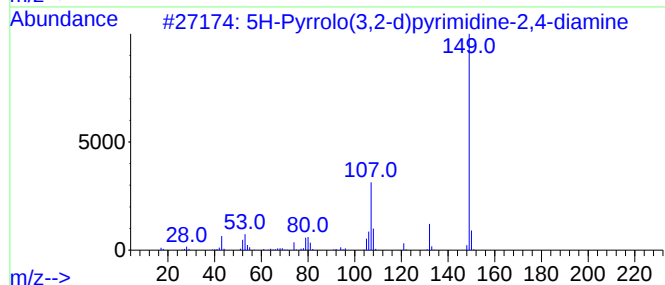
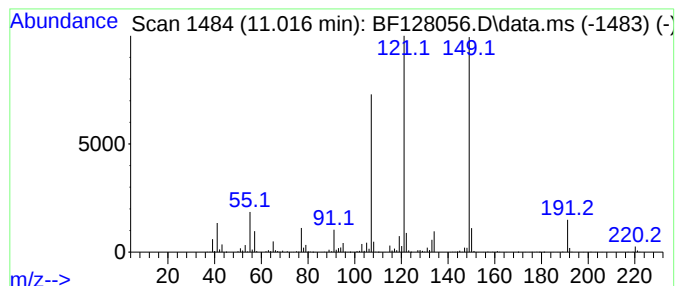
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown11.016 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.016	32.75 ng	1084320	Phenanthrene-d10	11.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5H-Pyrrolo(3,2-d)pyrimidine-2,4-...	149	C6H7N5	1000244-21-4	46
2			Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	38
3			Phenol, 2-methyl-4-(1,1,3,3-tetr...	220	C15H24O	002219-84-3	38
4			Methyl (1s,3s,5R,7S)-3-methylada...	208	C13H20O2	1010504-39-1	35
5			Phenol, 4-(1-methylpropyl)-	150	C10H14O	000099-71-8	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
Data File : BF128056.D
Acq On : 03 May 2022 20:09
Operator : CG\JU
Sample : N2659-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-D

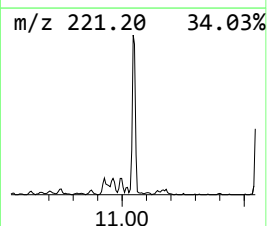
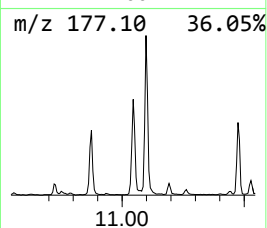
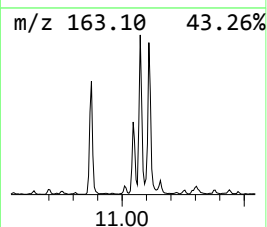
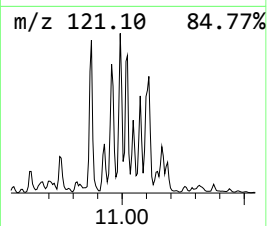
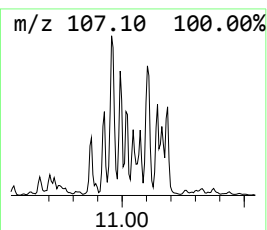
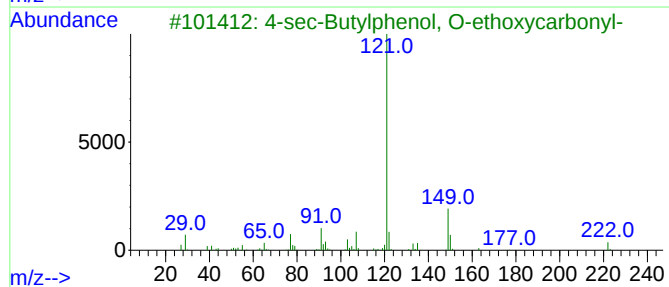
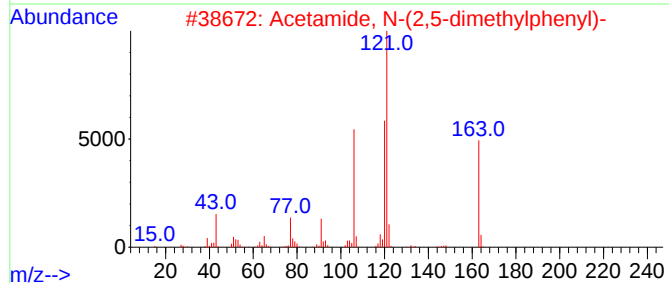
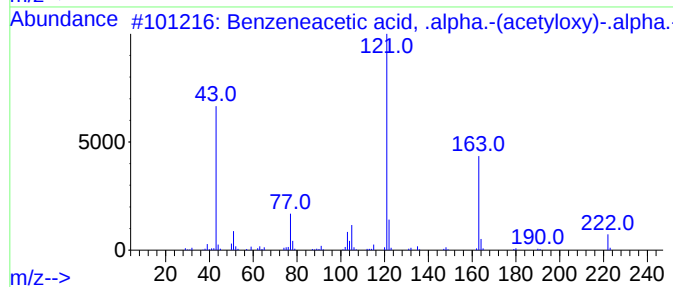
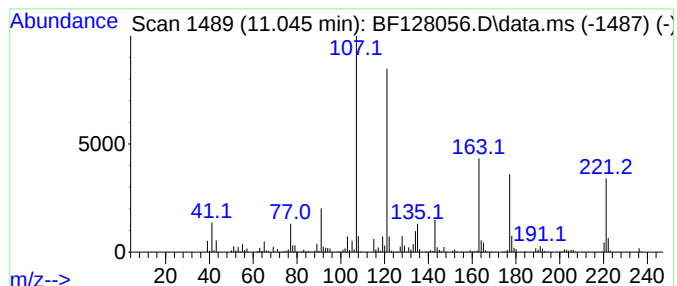
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown11.045 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.045	29.33 ng	971104	Phenanthrene-d10	11.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneacetic acid, .alpha.-(ace...	222	C12H14O4	055012-78-7	41
2			Acetamide, N-(2,5-dimethylphenyl)-	163	C10H13NO	002050-44-4	38
3			4-sec-Butylphenol, O-ethoxycarbo...	222	C13H18O3	1000487-30-7	35
4			1-(Isocyanatomethyl)-4-(methylox...	163	C9H9NO2	056651-60-6	35
5			Acetamide, N-(2,4-dimethylphenyl)-	163	C10H13NO	002050-43-3	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
Data File : BF128056.D
Acq On : 03 May 2022 20:09
Operator : CG\JU
Sample : N2659-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-D

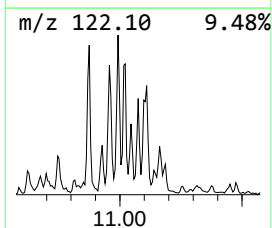
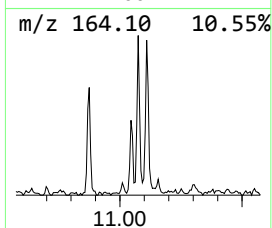
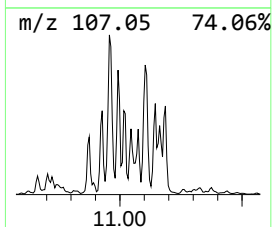
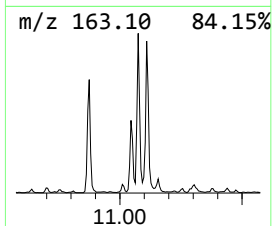
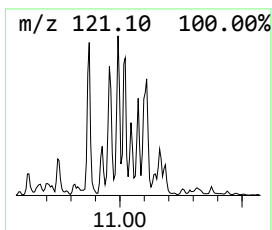
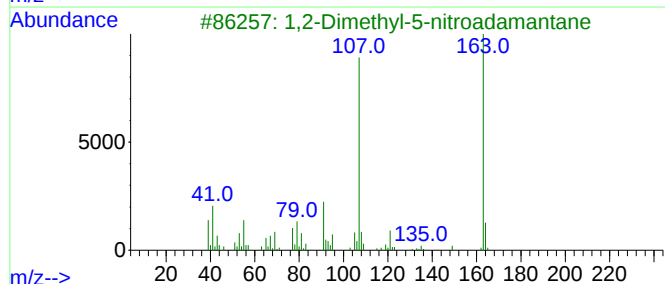
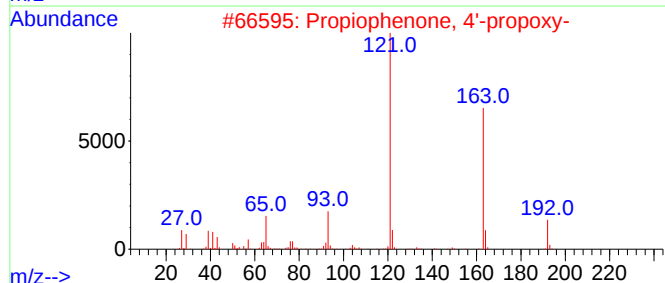
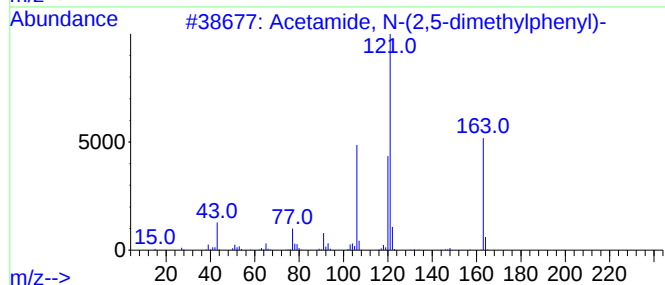
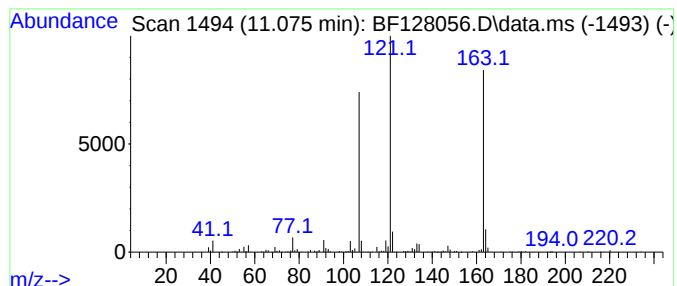
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Acetamide, N-(2,5-dimethylp... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.075	14.54 ng	481479	Phenanthrene-d10	11.451

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Acetamide, N-(2,5-dimethylphenyl)-	163	C10H13NO	002050-44-4	50
2		Propiophenone, 4'-propoxy-	192	C12H16O2	005736-87-8	47
3		1,2-Dimethyl-5-nitroadamantane	209	C12H19NO2	006588-68-7	38
4		N-Acetyl-L-tyrosinamide	222	C11H14N2O3	001948-71-6	38
5		2-Ethylphenol, isopropyl ether	164	C11H16O	1000395-15-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
Data File : BF128056.D
Acq On : 03 May 2022 20:09
Operator : CG\JU
Sample : N2659-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-D

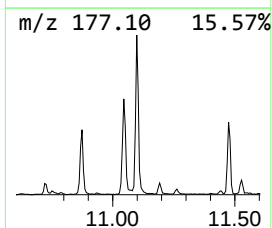
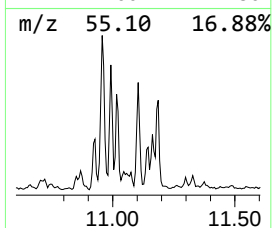
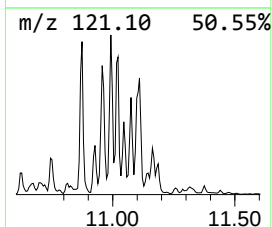
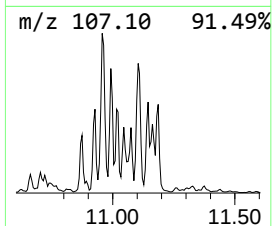
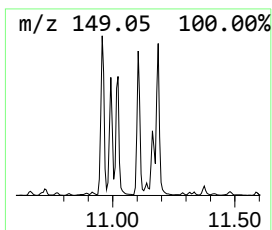
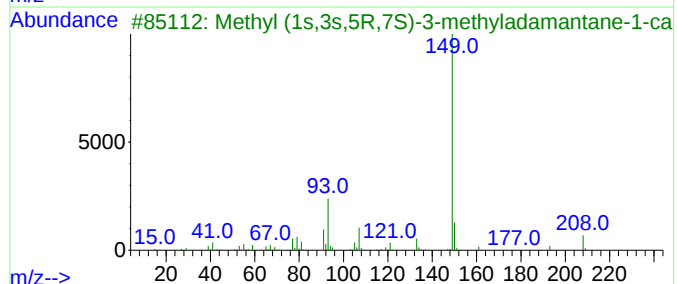
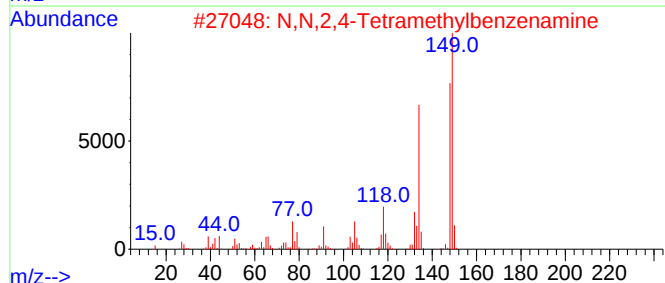
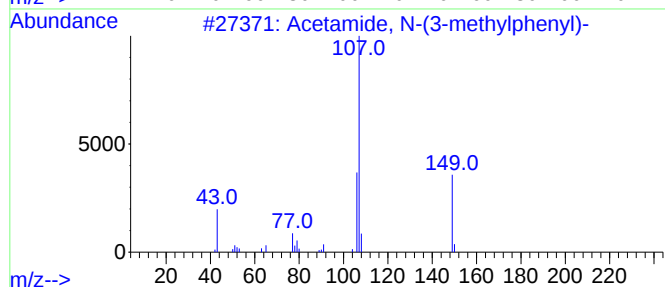
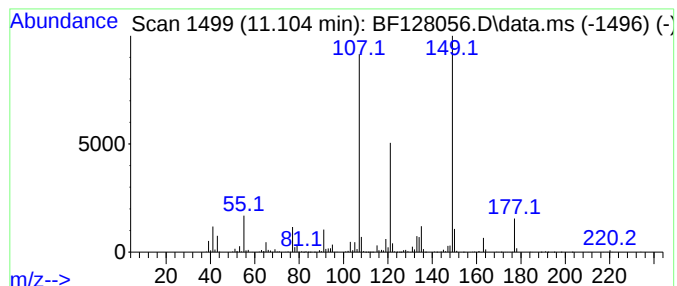
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Acetamide, N-(3-methylphenyl)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.104	57.71 ng	1910640	Phenanthrene-d10	11.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	64
2			N,N,2,4-Tetramethylbenzenamine	149	C10H15N	000769-53-9	38
3			Methyl (1s,3s,5R,7S)-3-methylada...	208	C13H20O2	1010504-39-1	38
4			3,4-(methylenedioxy)-phenylbutan...	192	C11H12O3	1000378-99-2	38
5			Phenol, 4-(2-methylpropyl)-	150	C10H14O	004167-74-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
Data File : BF128056.D
Acq On : 03 May 2022 20:09
Operator : CG\JU
Sample : N2659-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-D

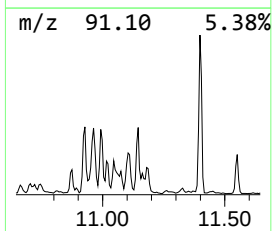
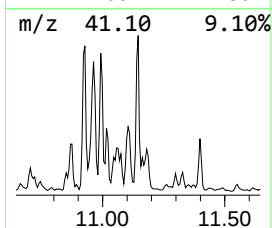
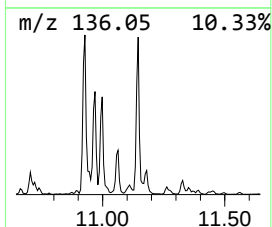
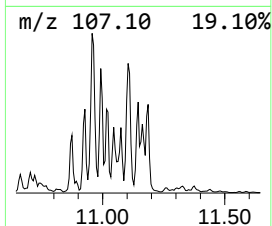
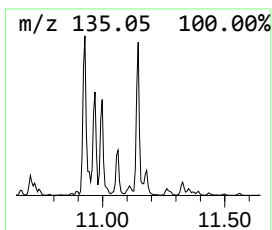
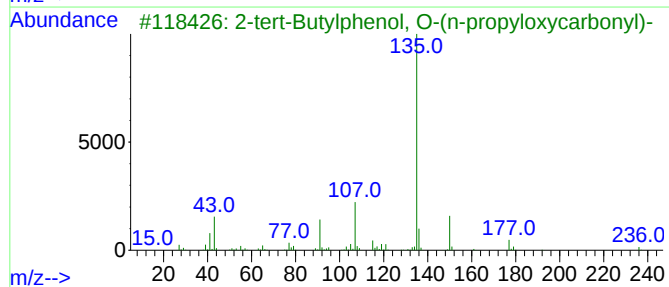
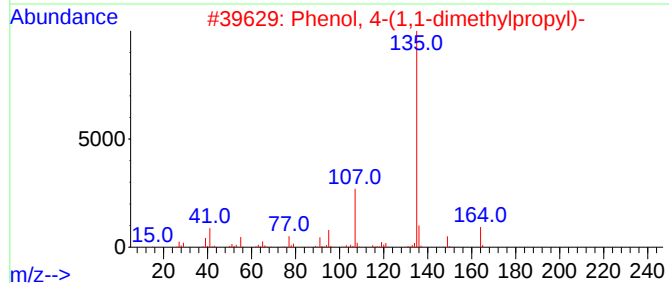
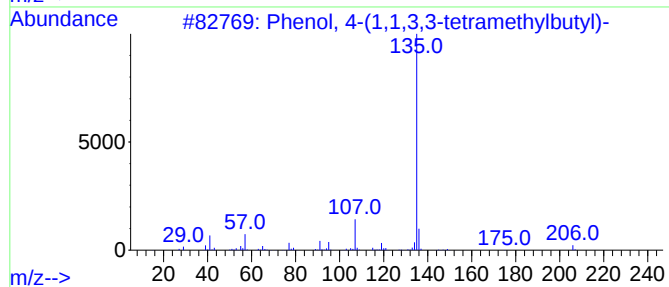
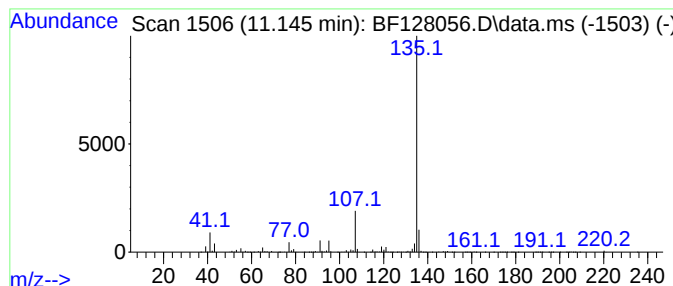
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 2-tert-Butylphenol, O-(n-pr... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.145	61.69 ng	2042400	Phenanthrene-d10	11.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	86
2			Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	83
3			2-tert-Butylphenol, O-(n-propylo...	236	C14H20O3	1000487-37-9	78
4			4-tert-Butylphenyl acetate	192	C12H16O2	003056-64-2	72
5			Phenol, 2-(1,1,3,3-tetramethylbu...	206	C14H22O	003884-95-5	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
Data File : BF128056.D
Acq On : 03 May 2022 20:09
Operator : CG\JU
Sample : N2659-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-D

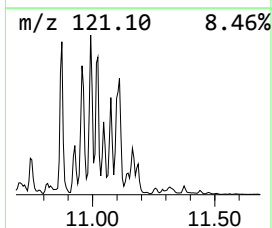
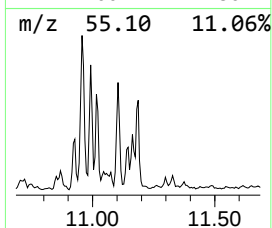
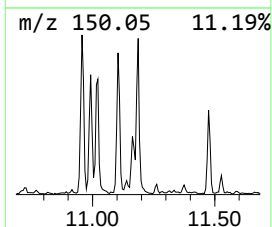
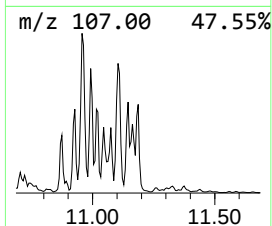
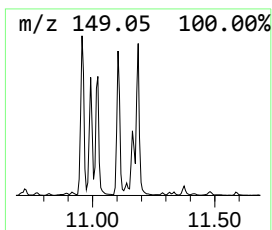
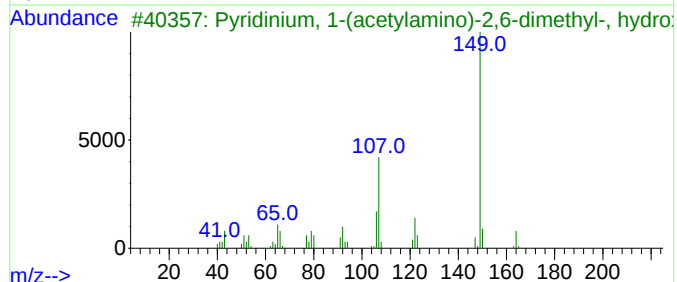
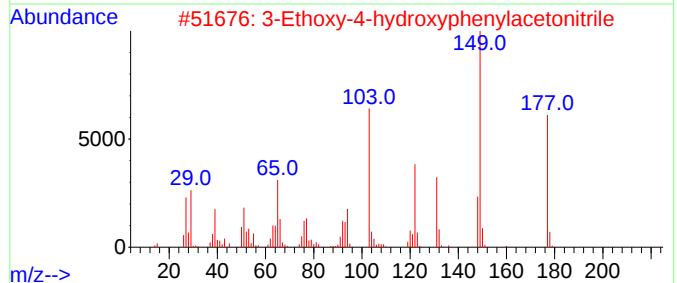
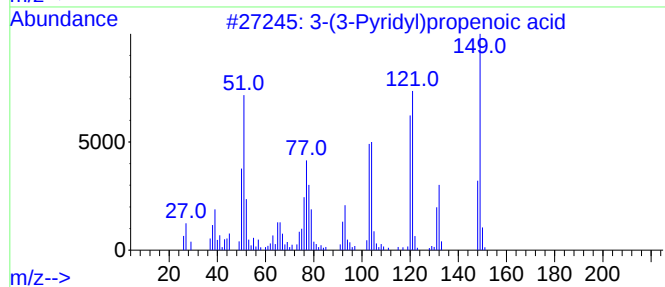
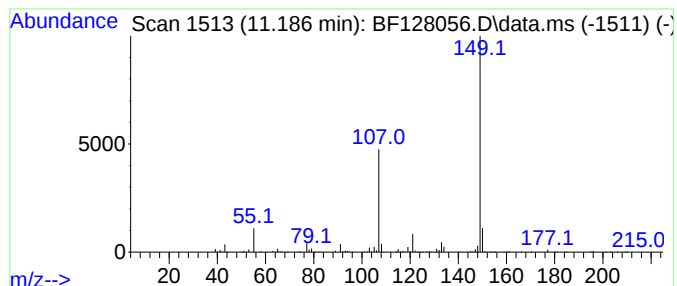
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown11.186 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.186	31.14 ng	1031030	Phenanthrene-d10	11.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-(3-Pyridyl)propenoic acid	149	C8H7NO2	001126-74-5	49
2			3-Ethoxy-4-hydroxyphenylacetoni...	177	C10H11NO2	205748-01-2	47
3			Pyridinium, 1-(acetylamino)-2,6-...	164	C9H12N2O	031020-35-6	43
4			N-(.alpha.-Methylbenzyl)-formamide	149	C9H11NO	006948-01-2	43
5			Phenol, 4-(1,1-dimethylethyl)-2-...	164	C11H16O	000098-27-1	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
Data File : BF128056.D
Acq On : 03 May 2022 20:09
Operator : CG\JU
Sample : N2659-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-D

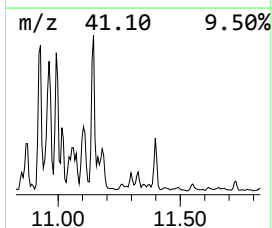
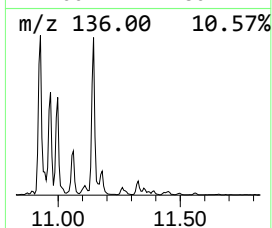
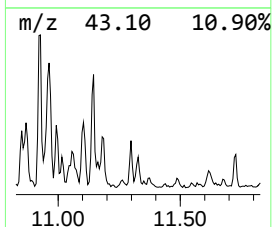
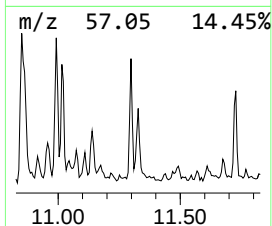
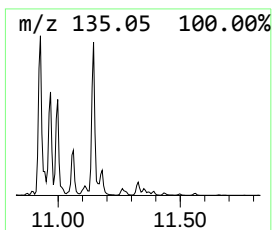
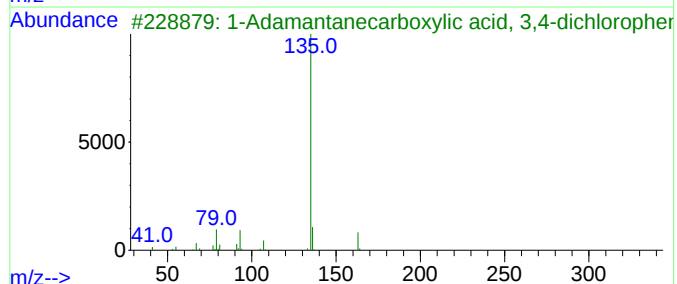
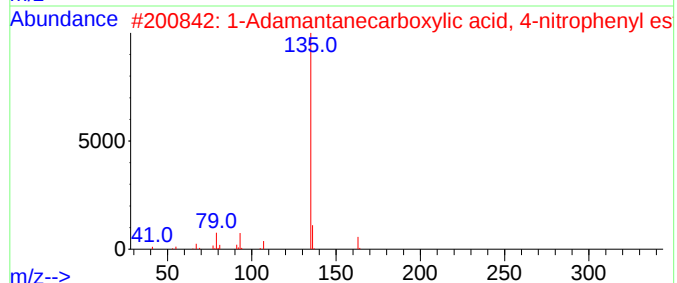
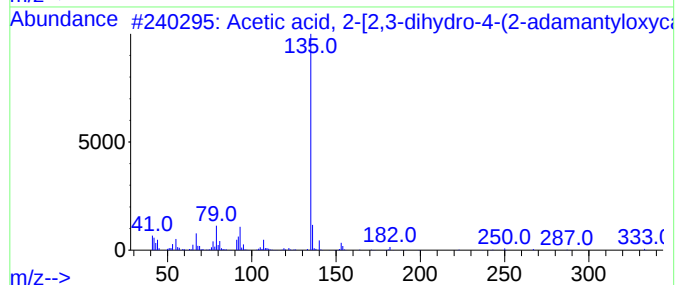
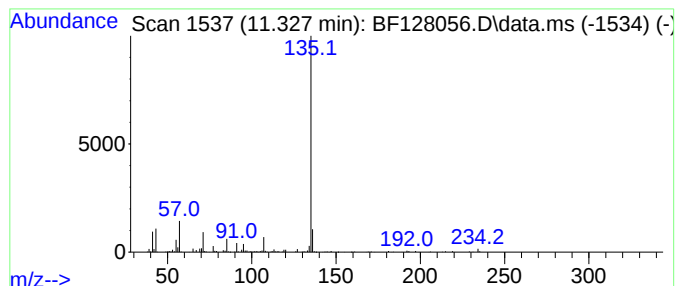
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Acetic acid, 2-[2,3-dihydro... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.327	8.10 ng	268097	Phenanthrene-d10	11.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 2-[2,3-dihydro-4-(2...	333	C18H23NO5	1000294-10-3	59
2			1-Adamantanecarboxylic acid, 4-n...	301	C17H19NO4	1000307-66-5	53
3			1-Adamantanecarboxylic acid, 3,4...	324	C17H18Cl2O2	1000307-66-4	53
4			1-Adamantanecarboxylic acid, 4-c...	290	C17H19ClO2	1000307-66-0	53
5			1-Ethyladamantane	164	C12H20	000770-69-4	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
Data File : BF128056.D
Acq On : 03 May 2022 20:09
Operator : CG\JU
Sample : N2659-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-D

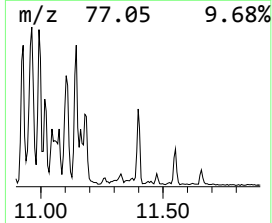
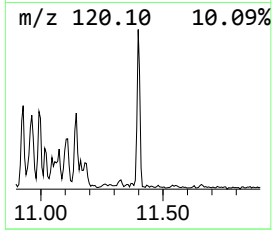
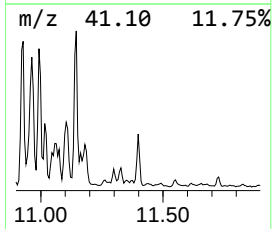
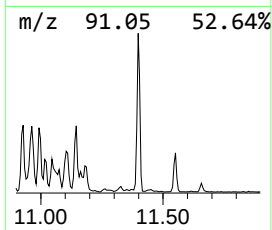
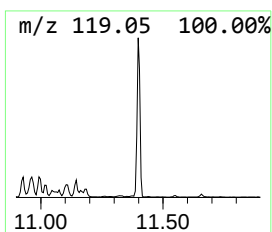
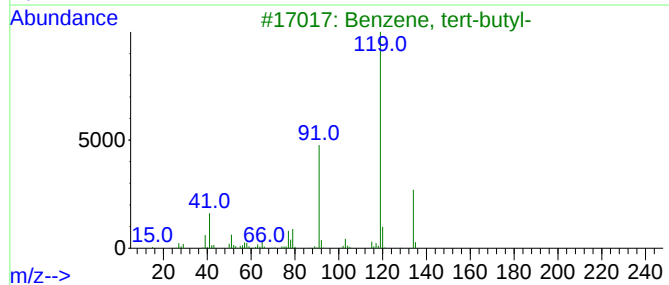
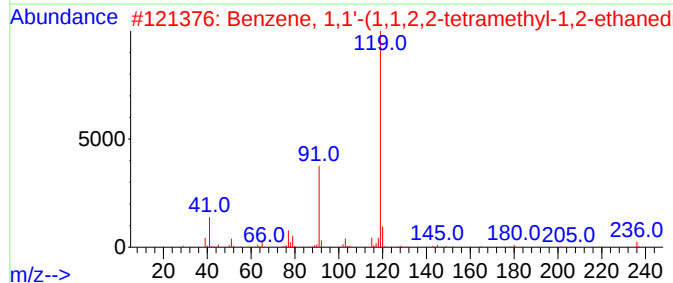
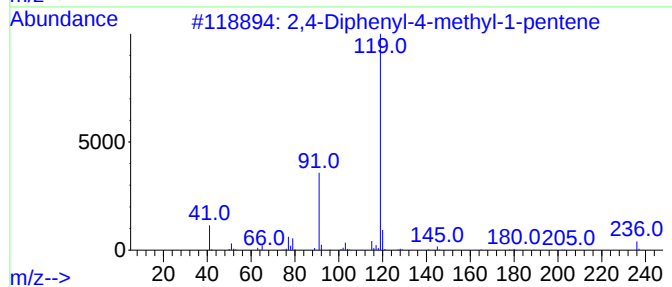
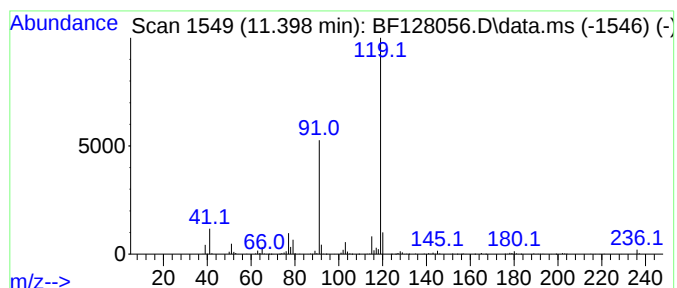
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 2,4-Diphenyl-4-methyl-1-pen... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.398	18.54 ng	613644	Phenanthrene-d10	11.451

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Diphenyl-4-methyl-1-pentene	236	C18H20	1000111-58-0	94	
2	Benzene, 1,1'-(1,1,2,2-tetrameth...	238	C18H22	001889-67-4	83	
3	Benzene, tert-butyl-	134	C10H14	000098-06-6	78	
4	2-Pentanone, 4-methyl-4-phenyl-	176	C12H16O	007403-42-1	78	
5	(6-Chloro-2-methylhexan-2-yl)ben...	210	C13H19Cl	1417621-45-4	78	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
Data File : BF128056.D
Acq On : 03 May 2022 20:09
Operator : CG\JU
Sample : N2659-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-D

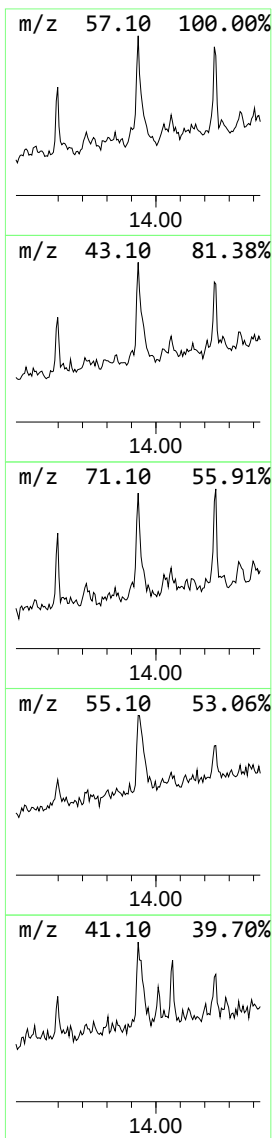
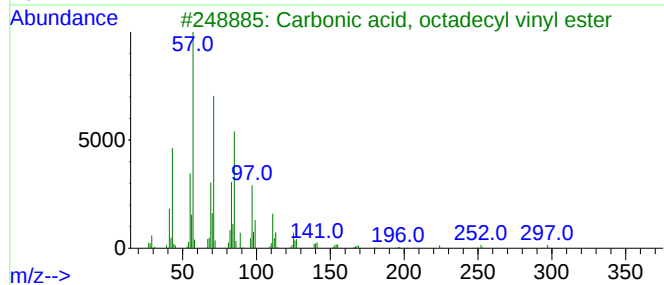
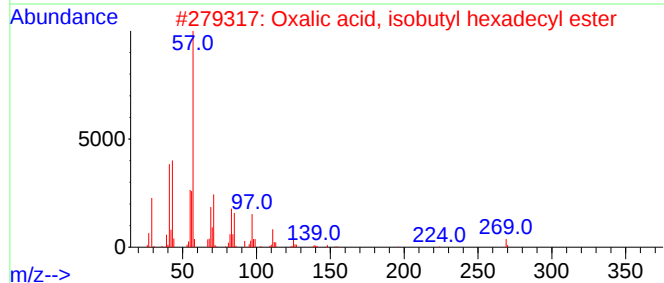
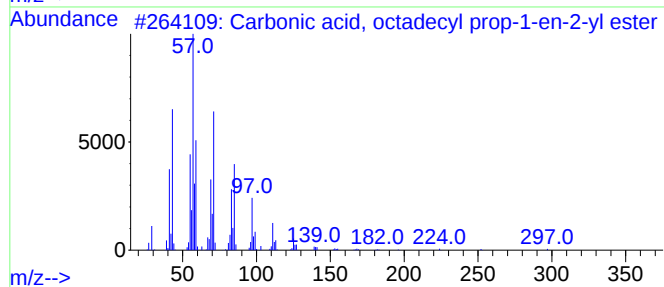
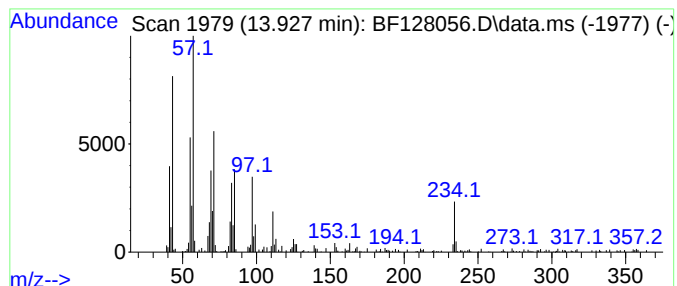
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Carbonic acid, octadecyl pr... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	7.88 ng	298139	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	81
2			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	74
3			Carbonic acid, octadecyl vinyl e...	340	C21H40O3	1000382-54-4	74
4			Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	74
5			Tridecane	184	C13H28	000629-50-5	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
Data File : BF128056.D
Acq On : 03 May 2022 20:09
Operator : CG\JU
Sample : N2659-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

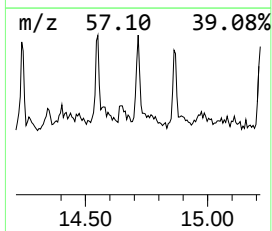
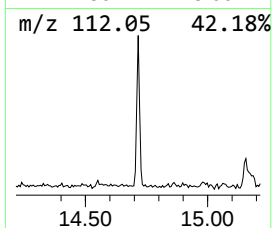
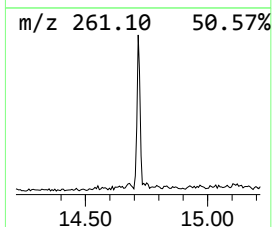
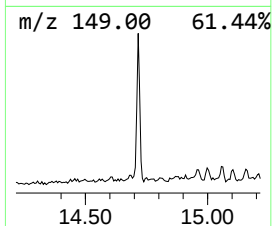
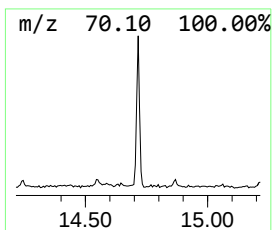
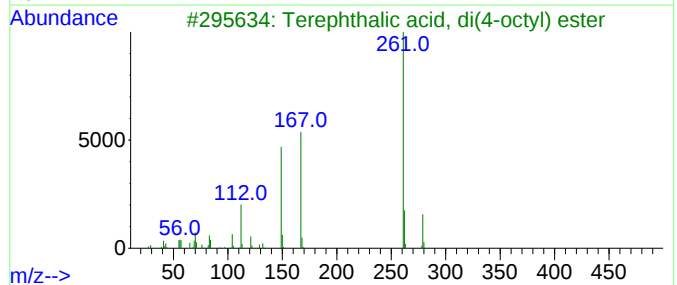
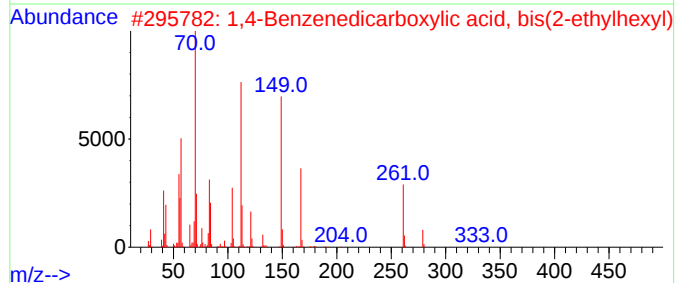
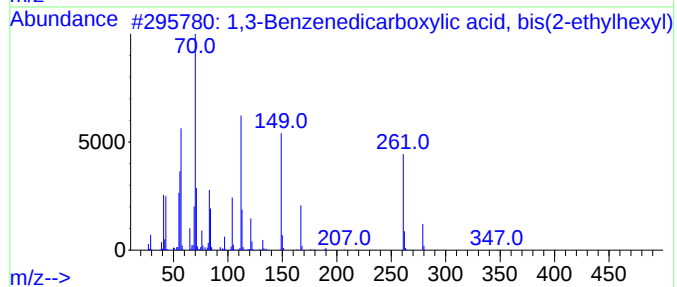
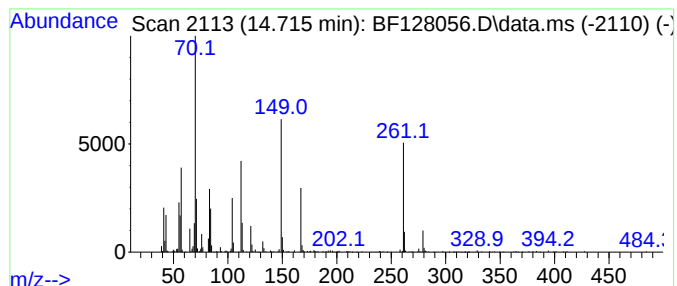
Instrument :
BNA_F
ClientSampleId :
22L097-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 1,3-Benzenedicarboxylic aci... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.716	6.34 ng	240078	Chrysene-d12	14.098	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	64
2	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	52
3	Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	43
4	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	43
5	Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
 Data File : BF128056.D
 Acq On : 03 May 2022 20:09
 Operator : CG\JU
 Sample : N2659-04
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 22L097-D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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-Pentanone, 4-...	5.169	162.8	ng	4715270	1	6.916	579431	20.0
Neopentyl glycol	6.175	28.2	ng	818053	1	6.916	579431	20.0
Ethanol, 2-(2-b...	8.104	60.7	ng	2266920	2	8.198	747125	20.0
2,4,7,9-Tetrame...	9.380	5.8	ng	234075	3	9.957	804709	20.0
Phenol, 4-(1,1-...	10.704	10.3	ng	342166	4	11.451	662139	20.0
Pivalic acid, 4...	10.745	6.9	ng	228999	4	11.451	662139	20.0
1-(Isocyanatome...	10.874	29.0	ng	960953	4	11.451	662139	20.0
Phenol, 4-(1,1,...	10.928	64.0	ng	2117700	4	11.451	662139	20.0
4-(7-Methylocty...	10.963	92.5	ng	3062330	4	11.451	662139	20.0
Phenol, p-tert-...	10.992	68.8	ng	2275940	4	11.451	662139	20.0
unknown11.016	11.016	32.8	ng	1084320	4	11.451	662139	20.0
unknown11.045	11.045	29.3	ng	971104	4	11.451	662139	20.0
Acetamide, N-(2...	11.075	14.5	ng	481479	4	11.451	662139	20.0
Acetamide, N-(3...	11.104	57.7	ng	1910640	4	11.451	662139	20.0
2-tert-Butylphe...	11.145	61.7	ng	2042400	4	11.451	662139	20.0
unknown11.186	11.186	31.1	ng	1031030	4	11.451	662139	20.0
Acetic acid, 2-...	11.327	8.1	ng	268097	4	11.451	662139	20.0
2,4-Diphenyl-4-...	11.398	18.5	ng	613644	4	11.451	662139	20.0
Carbonic acid, ...	13.927	7.9	ng	298139	5	14.098	756957	20.0
1,3-Benzenedica...	14.716	6.3	ng	240078	5	14.098	756957	20.0