

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092923\
 Data File : BF135516.D
 Acq On : 29 Sep 2023 15:12
 Operator : CG\JU
 Sample : 04645-02
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 02

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135516.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	13	17	32	rVB	304349	411217	5.36%	0.392%
2	3.375	196	219	249	rBV	518887	3815729	49.71%	3.634%
3	5.387	557	561	575	rBV	3946057	4191736	54.61%	3.992%
4	6.175	689	695	707	rBV3	39190	116624	1.52%	0.111%
5	6.316	716	719	723	rBV	88097	133675	1.74%	0.127%
6	6.404	730	734	759	rVB	3581402	4222591	55.01%	4.022%
7	6.592	764	766	777	rVB	79533	143257	1.87%	0.136%
8	6.745	789	792	799	rBV	1173929	981634	12.79%	0.935%
9	6.816	799	804	810	rBV2	128532	145514	1.90%	0.139%
10	7.157	858	862	865	rBV2	124062	126632	1.65%	0.121%
11	7.316	881	889	892	rBV	2751270	2742030	35.72%	2.611%
12	7.428	904	908	914	rBV2	71968	108046	1.41%	0.103%
13	7.492	915	919	925	rVV2	75153	123730	1.61%	0.118%
14	7.722	949	958	959	rBV4	403488	849454	11.07%	0.809%
15	7.739	959	961	976	rVB2	525168	992320	12.93%	0.945%
16	8.022	1006	1009	1012	rBV	1228127	1065680	13.88%	1.015%
17	8.051	1012	1014	1016	rVB2	210887	151559	1.97%	0.144%
18	8.286	1045	1054	1056	rBV2	392808	800151	10.42%	0.762%
19	8.304	1056	1057	1063	rVB	358109	312668	4.07%	0.298%
20	8.445	1078	1081	1083	rBV	93395	116041	1.51%	0.111%
21	8.675	1116	1120	1122	rVV	720427	934337	12.17%	0.890%
22	8.704	1122	1125	1132	rVV	1028014	2009971	26.18%	1.914%
23	8.781	1132	1138	1141	rVV	405238	967290	12.60%	0.921%
24	8.810	1141	1143	1153	rVB2	431743	671718	8.75%	0.640%
25	8.928	1160	1163	1165	rBV	211639	176991	2.31%	0.169%
26	8.951	1165	1167	1169	rVV	248584	199851	2.60%	0.190%
27	8.975	1169	1171	1180	rVB	669402	612939	7.98%	0.584%
28	9.045	1180	1183	1187	rVB3	99971	95468	1.24%	0.091%
29	9.104	1187	1193	1196	rVB	4271539	4499470	58.61%	4.285%
30	9.151	1196	1201	1203	rVB	169943	143896	1.87%	0.137%
31	9.222	1211	1213	1215	rVB	125990	94767	1.23%	0.090%
32	9.357	1232	1236	1237	rBV	365331	356554	4.64%	0.340%
33	9.381	1237	1240	1242	rVV	776423	760796	9.91%	0.725%
34	9.404	1242	1244	1247	rVV	451849	394256	5.14%	0.375%
35	9.439	1247	1250	1252	rVV	132129	135921	1.77%	0.129%
36	9.463	1252	1254	1258	rVV2	117116	124673	1.62%	0.119%

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37	9.533	1263	1266	1269	rVV	1563687	1269694	16.54%	1.209%
38	9.598	1273	1277	1280	rBV	1450974	1282028	16.70%	1.221%
39	9.780	1300	1308	1311	rBV	1291664	1244528	16.21%	1.185%
40	9.998	1343	1345	1348	rVV	208340	167159	2.18%	0.159%
41	10.045	1350	1353	1356	rVB	301346	262670	3.42%	0.250%
42	10.116	1360	1365	1372	rBV5	250036	396535	5.17%	0.378%
43	10.186	1372	1377	1378	rBV	671803	576241	7.51%	0.549%
44	10.204	1378	1380	1383	rVV	729151	593139	7.73%	0.565%
45	10.239	1383	1386	1395	rVV	728855	879670	11.46%	0.838%
46	10.369	1406	1408	1412	rBV	209563	180419	2.35%	0.172%
47	10.439	1414	1420	1423	rBV4	230157	376993	4.91%	0.359%
48	10.480	1423	1427	1432	rBV	2876442	3038028	39.58%	2.893%
49	10.533	1432	1436	1440	rBV	1430275	1292670	16.84%	1.231%
50	10.575	1440	1443	1446	rBV	1821841	1670757	21.76%	1.591%
51	10.710	1460	1466	1468	rBV4	755491	1370776	17.86%	1.306%
52	10.751	1471	1473	1476	rVV2	574029	681524	8.88%	0.649%
53	10.780	1476	1478	1482	rVB4	262581	280385	3.65%	0.267%
54	10.816	1482	1484	1486	rBV	128485	102419	1.33%	0.098%
55	10.869	1491	1493	1494	rBV2	199736	154269	2.01%	0.147%
56	10.951	1503	1507	1509	rBV2	507944	462117	6.02%	0.440%
57	10.980	1509	1512	1516	rVB2	193190	182257	2.37%	0.174%
58	11.045	1516	1523	1526	rBV	2114717	1994715	25.99%	1.900%
59	11.075	1526	1528	1534	rVV4	284397	287601	3.75%	0.274%
60	11.139	1537	1539	1541	rVV	170677	161538	2.10%	0.154%
61	11.169	1541	1544	1548	rVB	276072	294036	3.83%	0.280%
62	11.227	1551	1554	1557	rVB3	165323	152749	1.99%	0.145%
63	11.275	1558	1562	1564	rBV	982989	905445	11.80%	0.862%
64	11.298	1564	1566	1569	rVB	195829	146450	1.91%	0.139%
65	11.386	1577	1581	1584	rBV2	459932	522737	6.81%	0.498%
66	11.439	1587	1590	1593	rBV	634549	668139	8.70%	0.636%
67	11.569	1609	1612	1616	rBV2	179897	172395	2.25%	0.164%
68	11.616	1617	1620	1622	rBV2	147526	192387	2.51%	0.183%
69	11.657	1622	1627	1632	rBV2	639585	926743	12.07%	0.883%
70	11.739	1632	1641	1644	rBV2	2386763	7212349	93.95%	6.869%
71	11.774	1644	1647	1649	rVV3	1034734	1743202	22.71%	1.660%
72	11.822	1652	1655	1657	rVV	2378096	2688867	35.03%	2.561%
73	11.845	1657	1659	1661	rVB	1376072	1018781	13.27%	0.970%
74	11.910	1661	1670	1673	rBV6	382037	892013	11.62%	0.850%
75	11.974	1679	1681	1684	rVB	303835	264589	3.45%	0.252%
76	12.198	1716	1719	1726	rBV2	643420	1058767	13.79%	1.008%

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77	12.257	1726	1729	1733	rVB3	174137	217617	2.83%	0.207%
78	12.327	1738	1741	1744	rBV4	203433	284145	3.70%	0.271%
79	12.392	1749	1752	1755	rVB2	277025	213737	2.78%	0.204%
80	12.421	1755	1757	1765	rVB2	409193	529823	6.90%	0.505%
81	12.510	1767	1772	1773	rBV2	1298449	1532464	19.96%	1.459%
82	12.539	1773	1777	1785	rVB2	2126439	2955340	38.50%	2.815%
83	12.621	1785	1791	1800	rBV2	4693207	7676401	100.00%	7.311%
84	12.692	1800	1803	1808	rBV2	1564415	1803475	23.49%	1.718%
85	12.739	1809	1811	1814	rBV2	439761	579051	7.54%	0.551%
86	12.869	1830	1833	1837	rVB	2519458	2669667	34.78%	2.543%
87	13.351	1911	1915	1917	rBV	1505425	1356263	17.67%	1.292%
88	13.410	1923	1925	1927	rVB	298680	210937	2.75%	0.201%
89	13.439	1927	1930	1933	rBV2	673346	607063	7.91%	0.578%
90	13.598	1955	1957	1959	rVB2	186848	132601	1.73%	0.126%
91	13.651	1963	1966	1968	rBV3	396119	494238	6.44%	0.471%
92	13.692	1970	1973	1975	rBV2	356465	512079	6.67%	0.488%
93	13.916	2007	2011	2017	rVB2	4636316	5573742	72.61%	5.308%
94	14.057	2032	2035	2038	rBV	627038	627295	8.17%	0.597%
95	14.327	2077	2081	2085	rVB2	2391001	2275022	29.64%	2.167%
96	14.527	2113	2115	2118	rBV2	438401	541370	7.05%	0.516%
97	14.563	2118	2121	2125	rVB2	633162	769038	10.02%	0.732%
98	14.774	2154	2157	2162	rVB2	323112	356595	4.65%	0.340%
99	15.398	2259	2263	2269	rBV	586208	1097363	14.30%	1.045%
100	17.404	2600	2604	2622	rVB	196772	487070	6.35%	0.464%

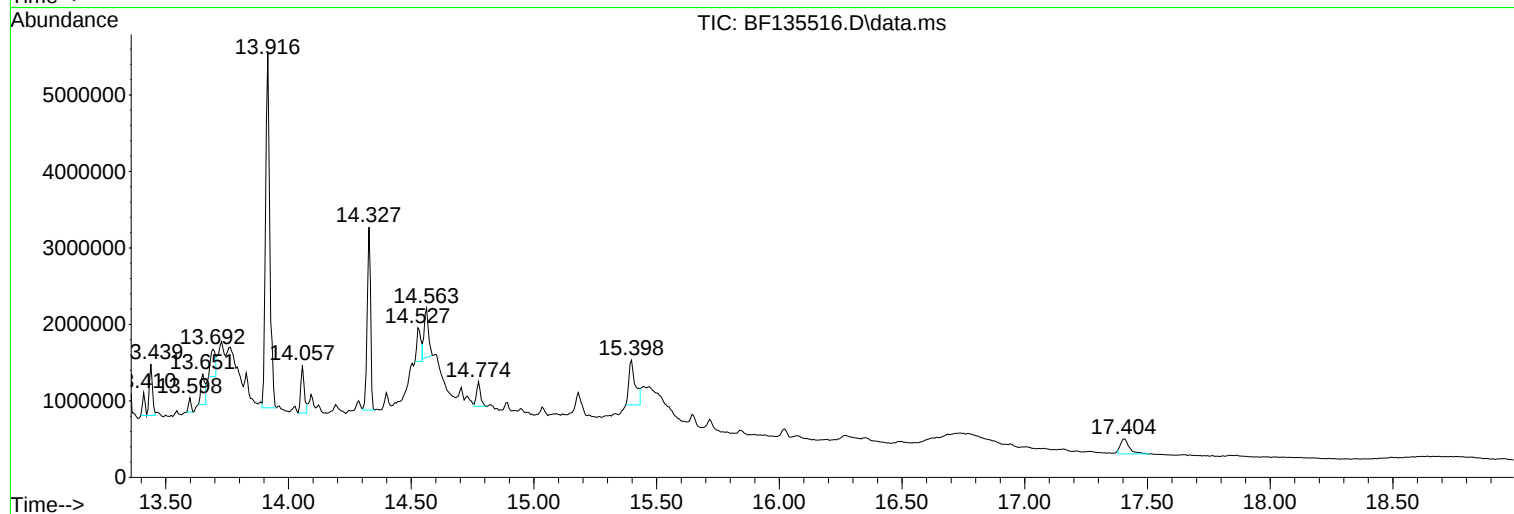
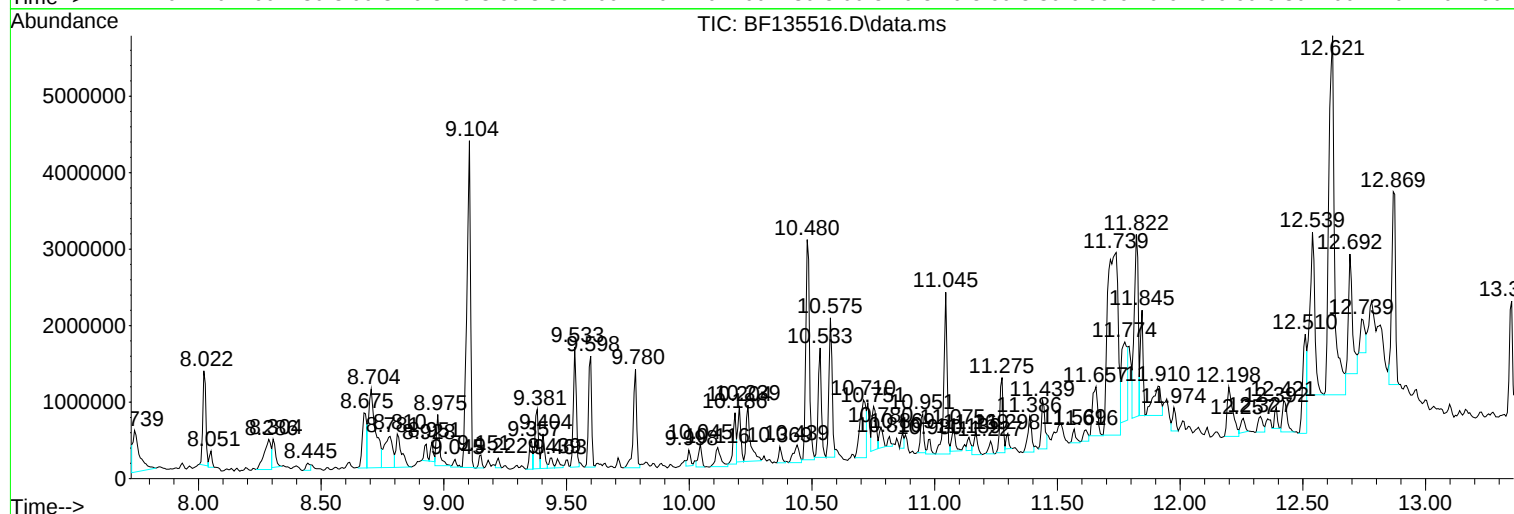
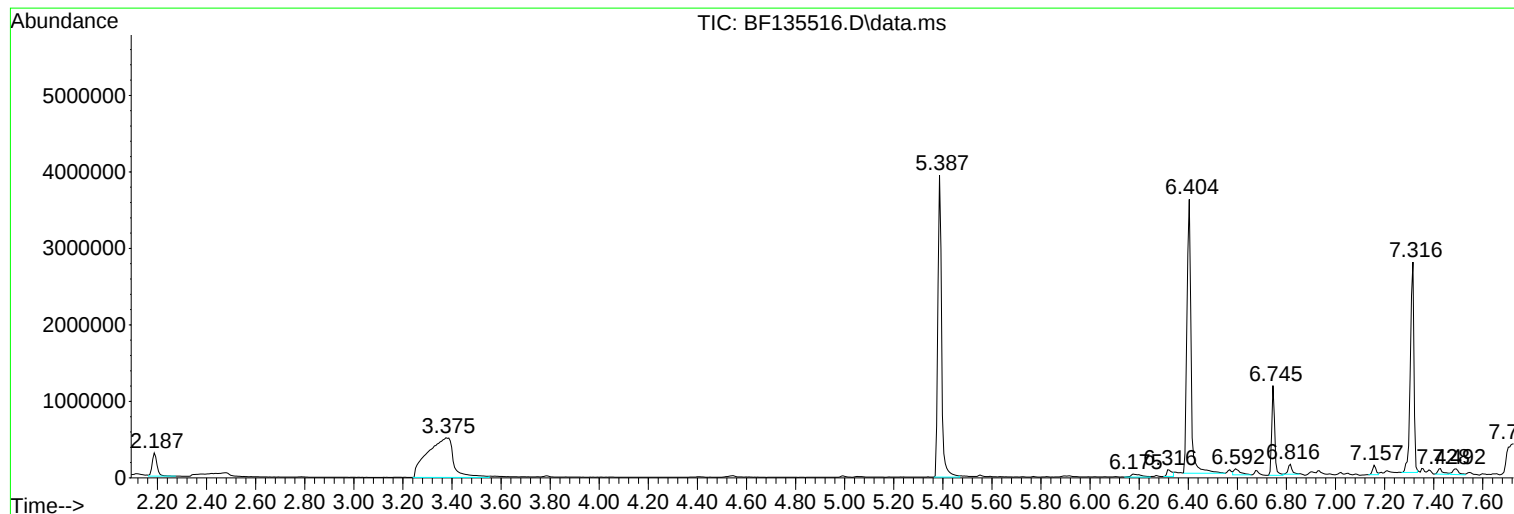
Sum of corrected areas: 104999363

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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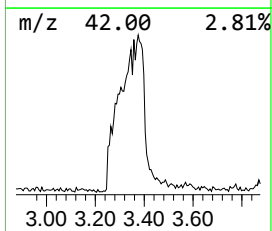
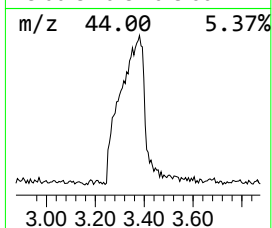
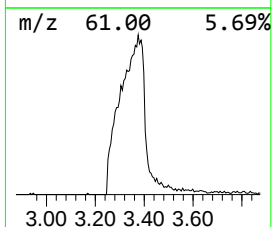
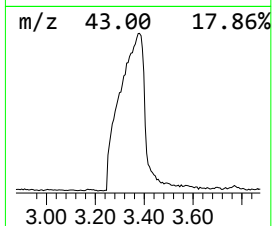
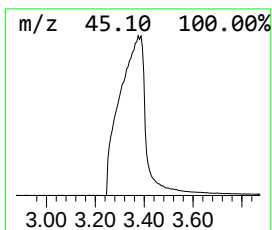
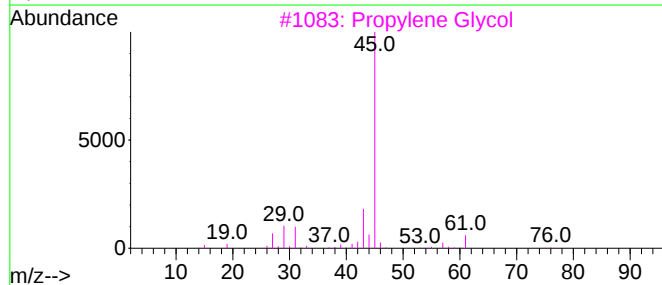
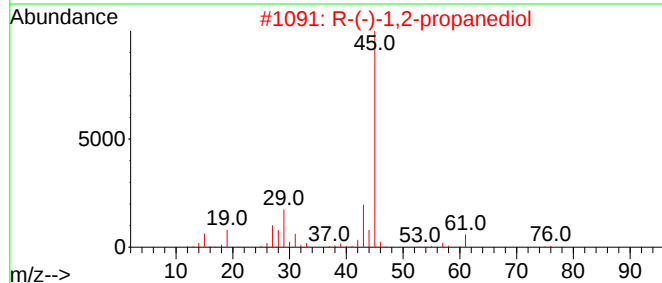
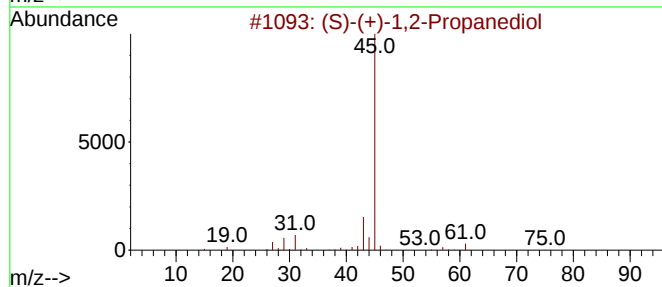
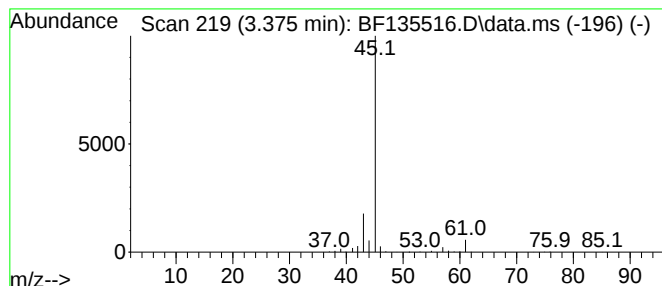
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.375	77.74 ng	3815730	1,4-Dichlorobenzene-d4	6.745

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
3		Propylene Glycol	76	C3H8O2	000057-55-6	43
4		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5		Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9



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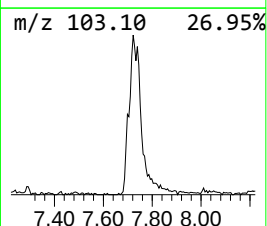
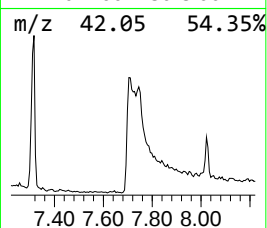
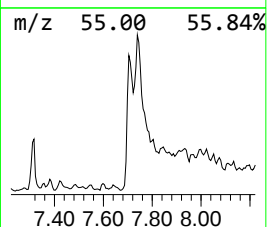
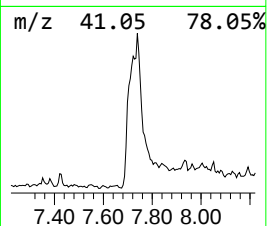
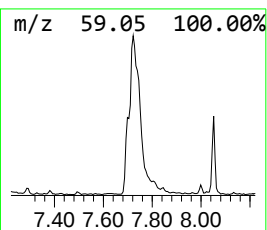
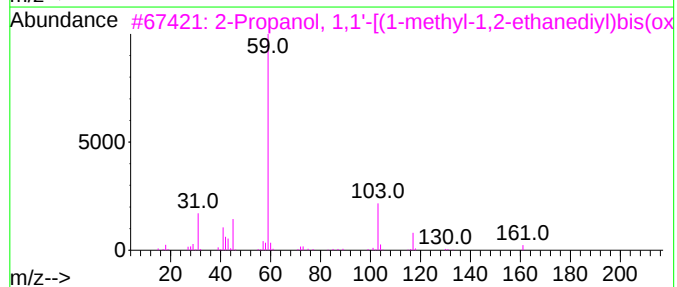
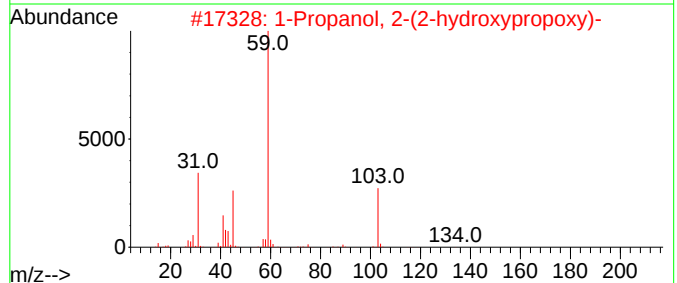
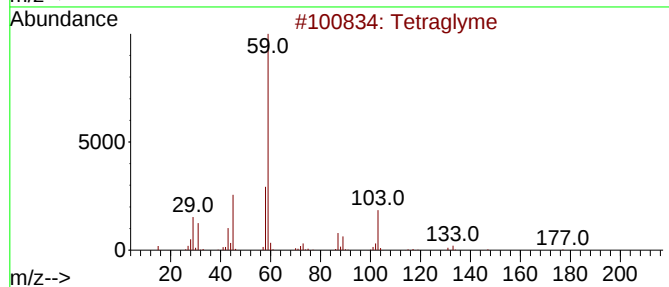
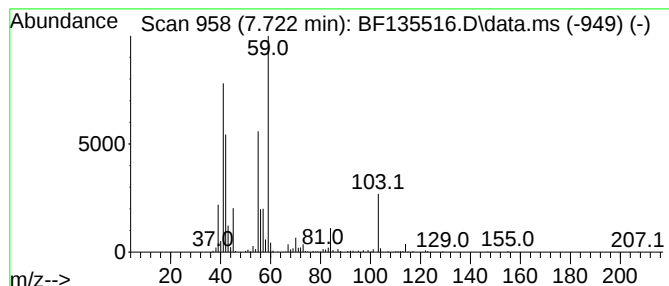
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.722 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.722	15.94 ng	849454	Naphthalene-d8	8.022

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetraglyme	222	C10H22O5	000143-24-8	47
2		1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	47
3		2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	43
4		Propanenitrile, 3-ethoxy-	99	C5H9NO	002141-62-0	43
5		2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	38



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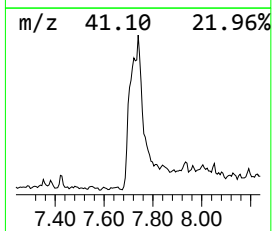
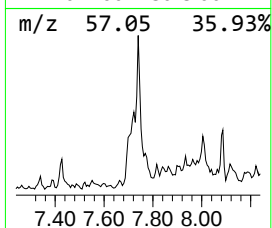
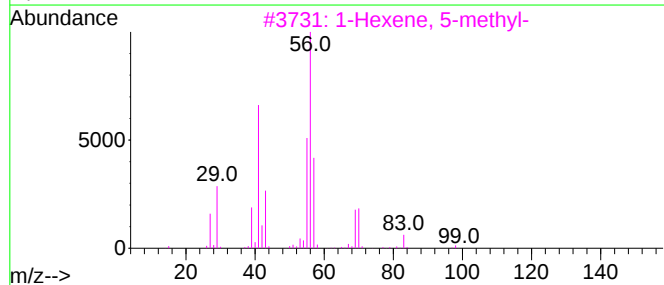
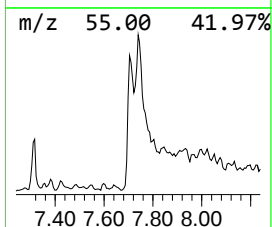
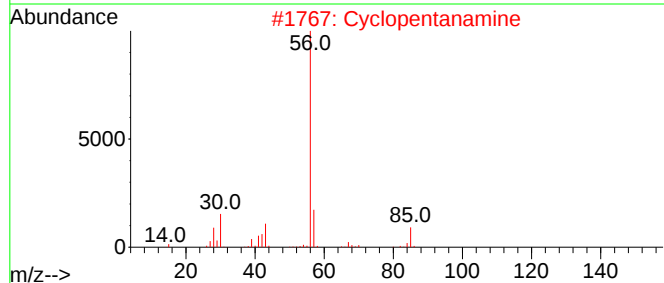
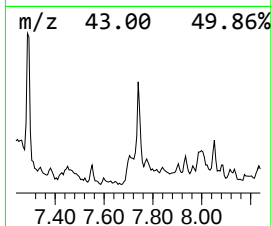
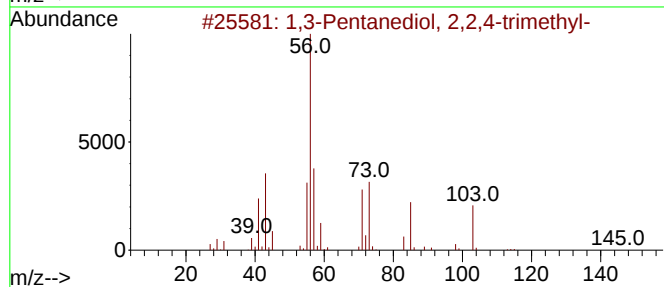
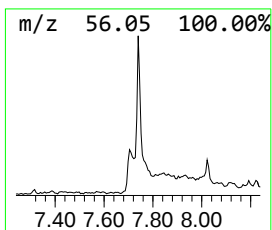
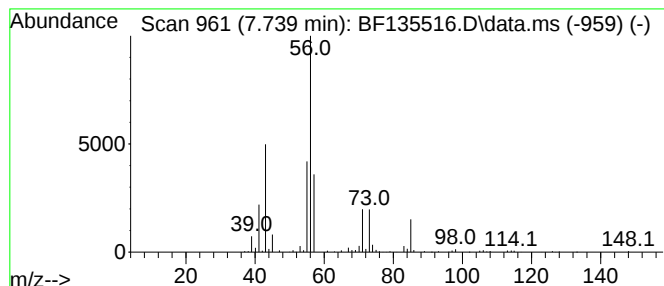
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 1,3-Pentanediol, 2,2,4-trim... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.739	18.62 ng	992320	Naphthalene-d8	8.022

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	50	
2	Cyclopentanamine	85	C5H11N	001003-03-8	38	
3	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	28	
4	1-Hexanol	102	C6H14O	000111-27-3	28	
5	Hexyl trifluoroacetate	198	C8H13F3O2	000400-61-3	25	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092923\
Data File : BF135516.D
Acq On : 29 Sep 2023 15:12
Operator : CG\JU
Sample : 04645-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

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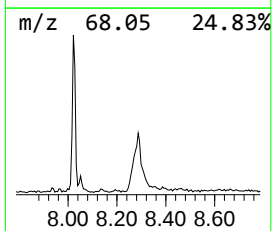
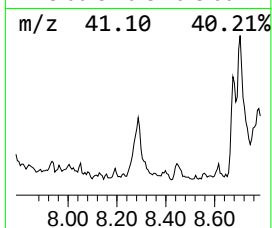
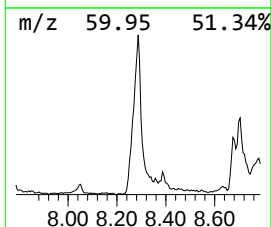
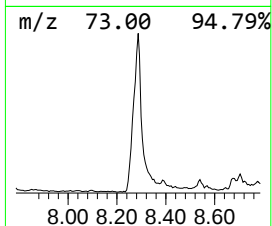
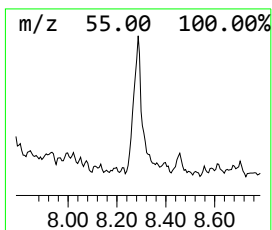
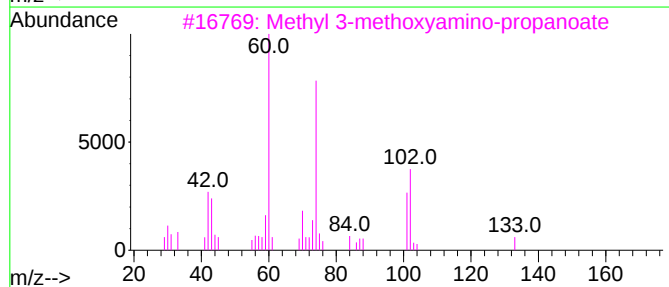
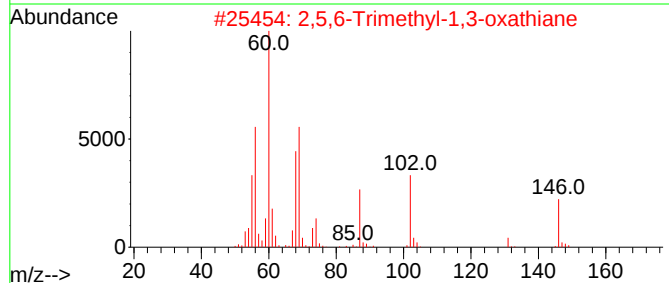
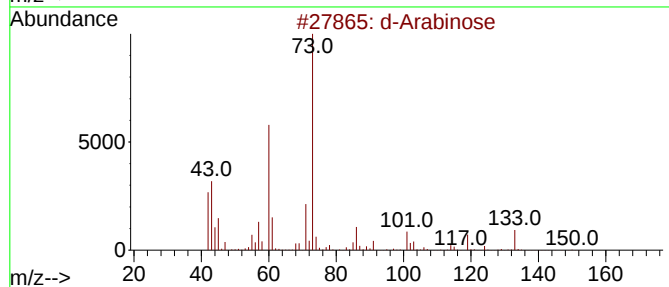
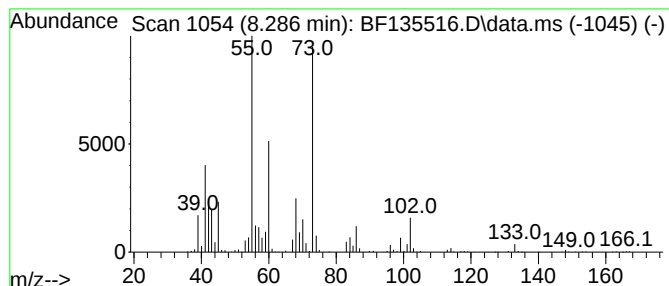
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown8.286 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.286	15.02 ng	800151	Naphthalene-d8	8.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	d-Arabinose			150	C5H10O5	010323-20-3	43
2	2,5,6-Trimethyl-1,3-oxathiane			146	C7H14OS	114376-06-6	38
3	Methyl 3-methoxyamino-propanoate			133	C5H11NO3	078191-05-6	38
4	DL-Arabinose			150	C5H10O5	020235-19-2	37
5	.alpha.-d-6,3-Furanose, methyl-....			192	C7H12O6	1000149-62-6	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092923\
Data File : BF135516.D
Acq On : 29 Sep 2023 15:12
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Sample : 04645-02
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Instrument :
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ClientSampleId :
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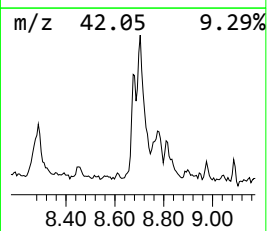
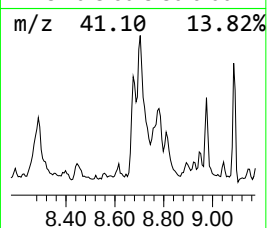
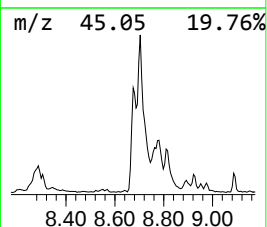
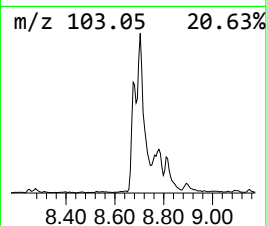
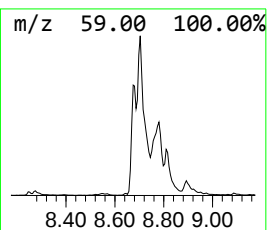
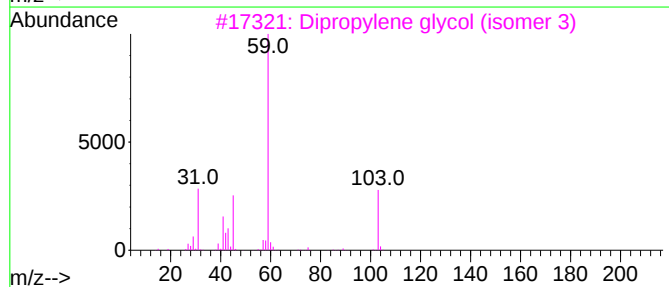
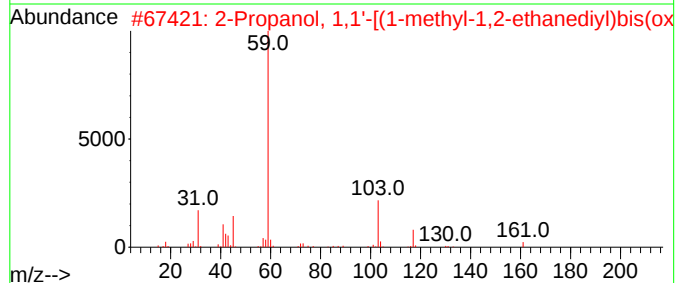
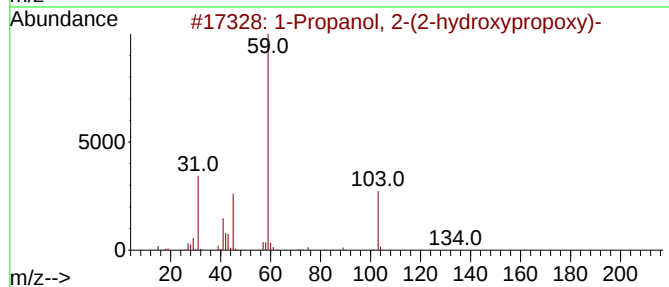
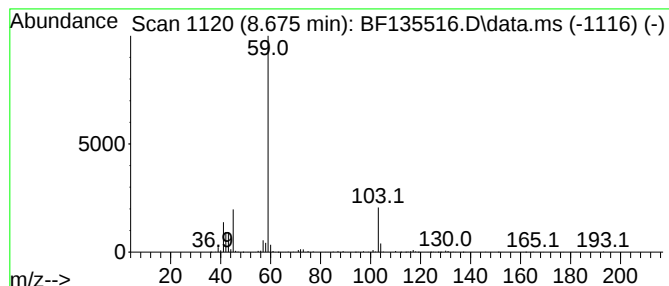
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Propanol, 2-(2-hydroxypro... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.675	17.54 ng	934337	Naphthalene-d8	8.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	83		
2	2-Propanol, 1,1'-[(1-methyl-1,2-...]	192	C9H20O4	001638-16-0	78		
3	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	74		
4	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	74		
5	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	74		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092923\
Data File : BF135516.D
Acq On : 29 Sep 2023 15:12
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Sample : 04645-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

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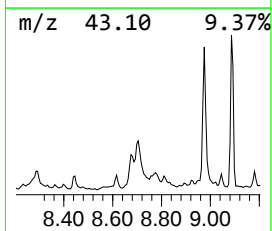
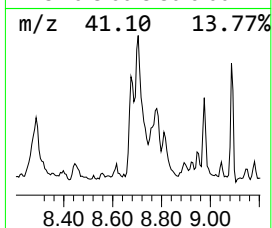
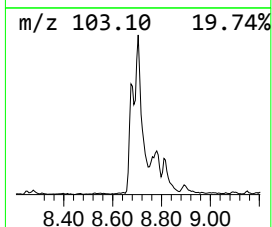
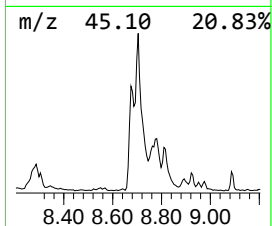
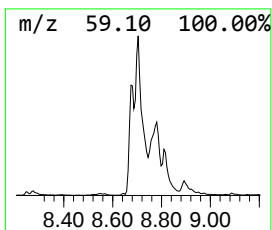
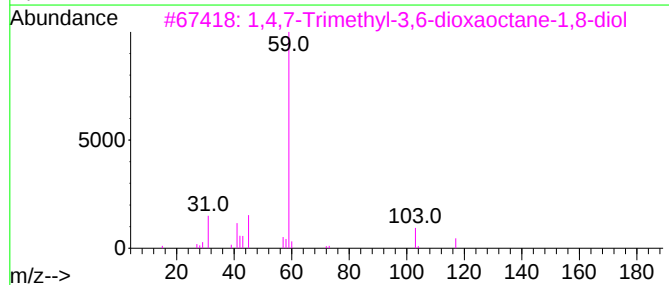
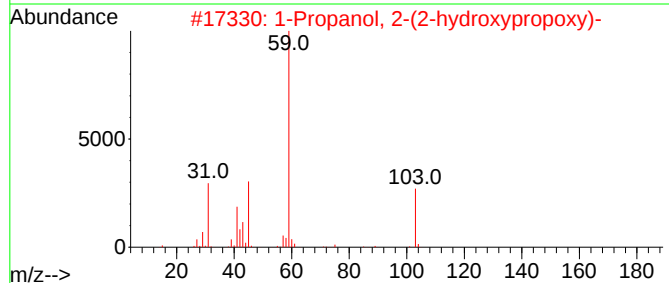
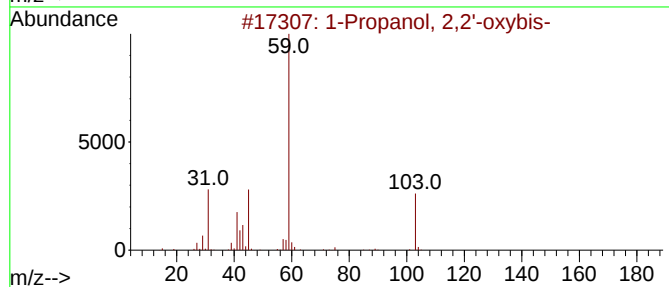
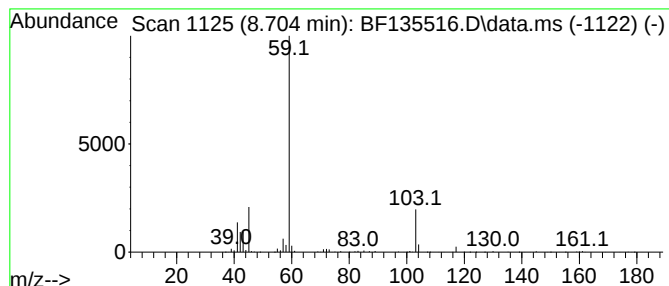
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Propanol, 2,2'-oxybis- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.704	37.72 ng	2009970	Naphthalene-d8	8.022

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	78
2		1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
3		1,4,7-Trimethyl-3,6-dioxaoctane-...	192	C9H20O4	1000423-63-2	56
4		2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	50
5		Hexaethylene glycol dimethyl ether	310	C14H30O7	001072-40-8	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092923\
Data File : BF135516.D
Acq On : 29 Sep 2023 15:12
Operator : CG\JU
Sample : 04645-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

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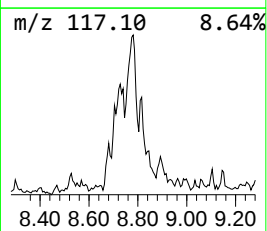
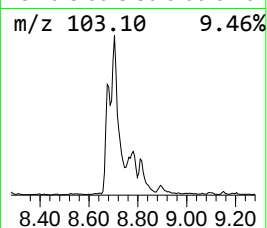
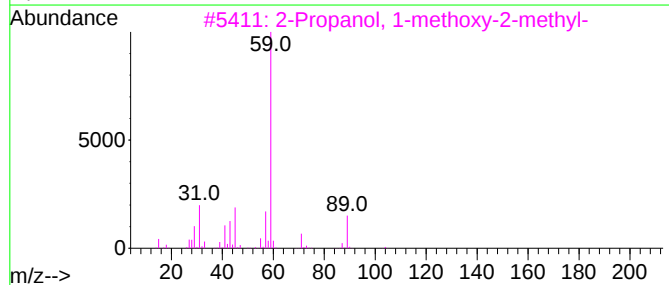
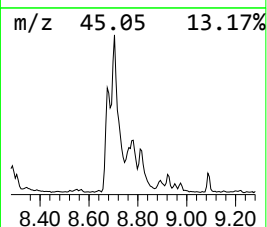
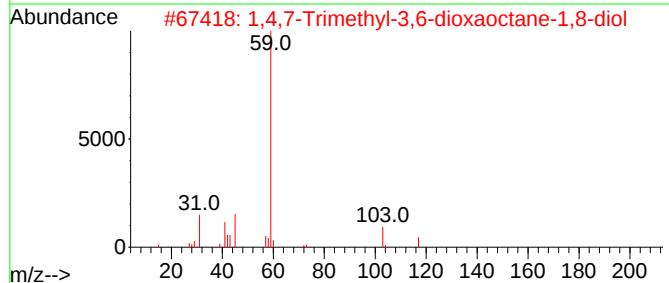
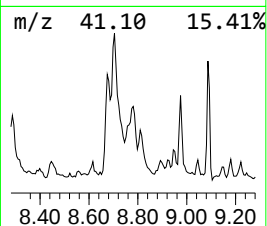
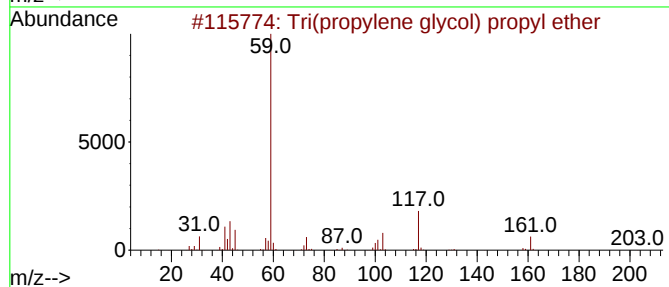
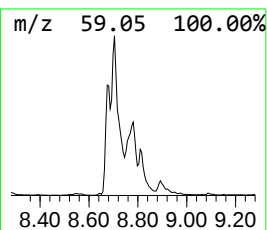
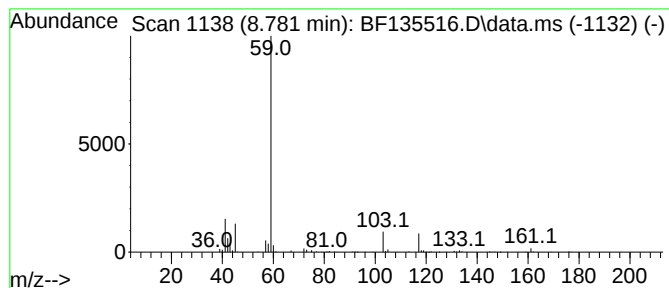
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tri(propylene glycol) propyl... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.781	18.15 ng	967290	Naphthalene-d8	8.022

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tri(propylene glycol) propyl ether	234	C12H26O4	096077-04-2	83
2		1,4,7-Trimethyl-3,6-dioxaoctane-...	192	C9H20O4	1000423-63-2	78
3		2-Propanol, 1-methoxy-2-methyl-	104	C5H12O2	003587-64-2	64
4		2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	56
5		Tetraglyme	222	C10H22O5	000143-24-8	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092923\
Data File : BF135516.D
Acq On : 29 Sep 2023 15:12
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Sample : 04645-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

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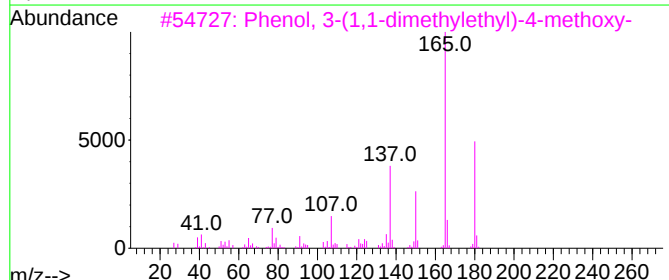
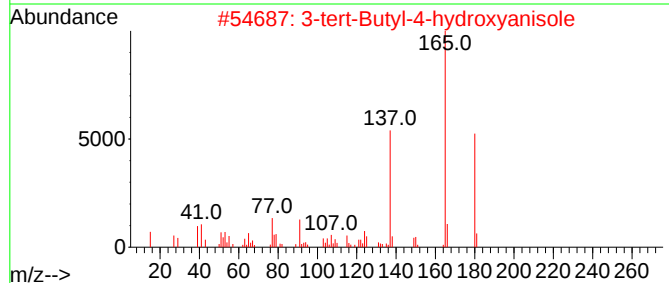
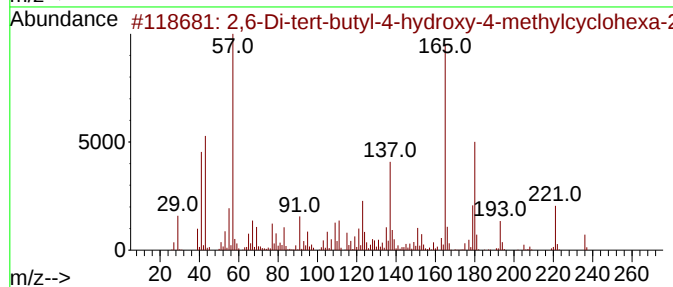
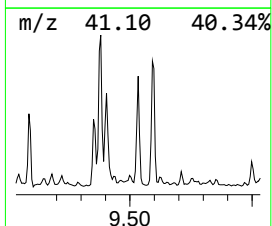
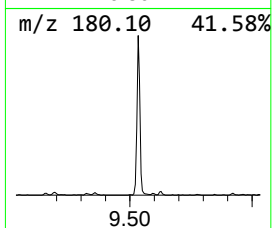
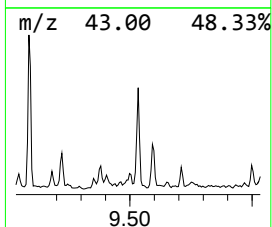
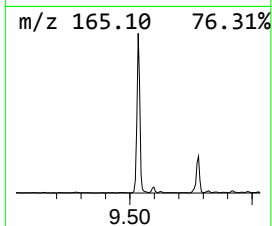
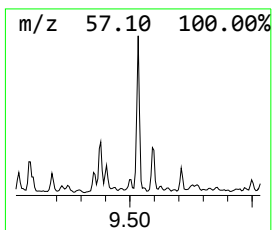
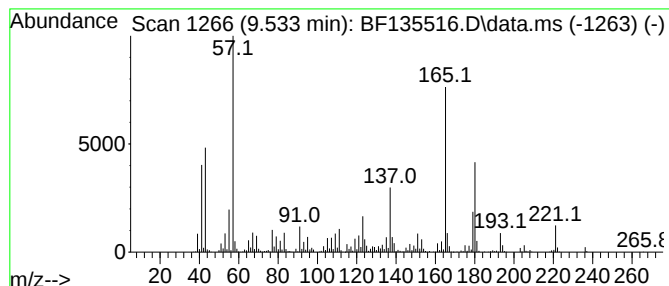
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2,6-Di-tert-butyl-4-hydroxy... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.533	20.40 ng	1269690	Acenaphthene-d10	9.780

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,6-Di-tert-butyl-4-hydroxy-4-me...	236	C15H24O2	010396-80-2	90
2			3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	83
3			Phenol, 3-(1,1-dimethylethyl)-4-...	180	C11H16O2	000088-32-4	70
4			Thiazolo[5,4-d]pyrimidine, 5-(et...	180	C7H8N4S	019835-21-3	50
5			Ethanone, 1-(2,5-dimethoxyphenyl)-	180	C10H12O3	001201-38-3	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092923\
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Misc :
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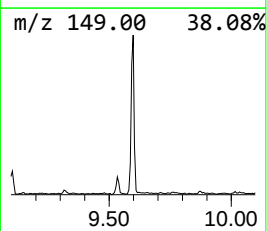
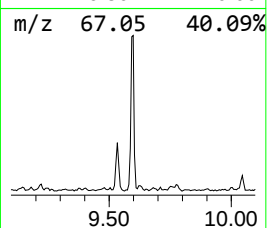
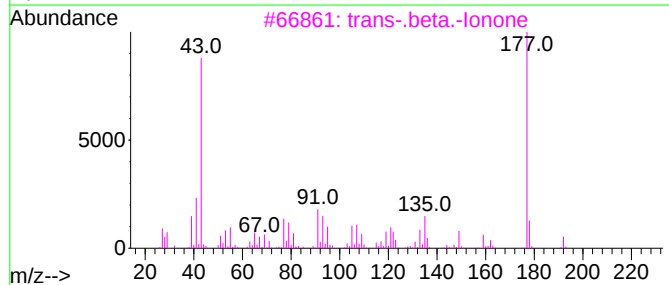
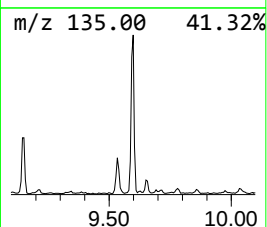
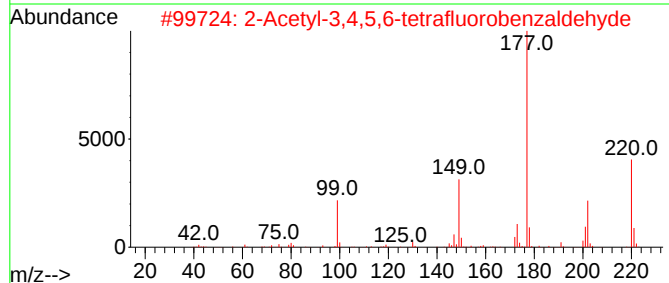
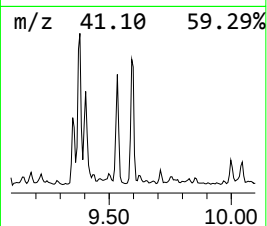
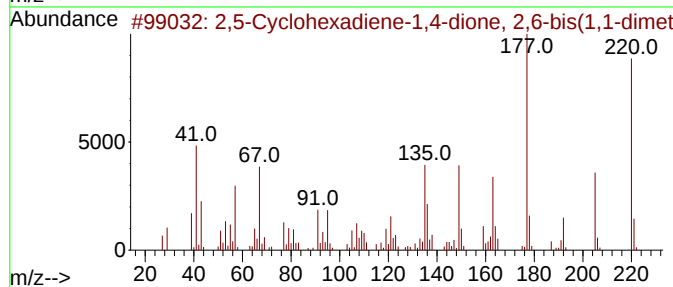
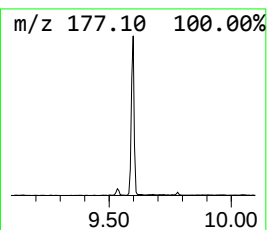
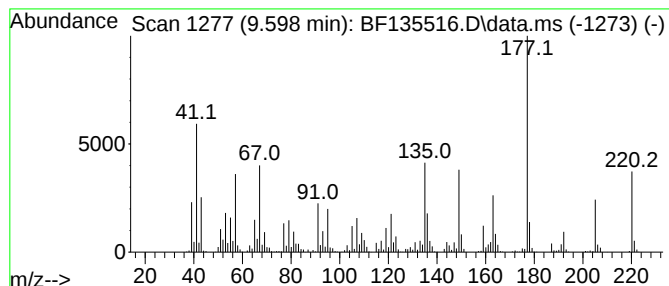
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.598	20.60 ng	1282030	Acenaphthene-d10	9.780	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	99
2	2-Acetyl-3,4,5,6-tetrafluorobenz...	220	C9H4F4O2	1000461-12-2	38
3	trans-.beta.-Ionone	192	C13H20O	000079-77-6	38
4	1,3,5,7-Tetramethyl-adamantane	192	C14H24	001687-36-1	38
5	2-Butanone, 3-(4-tert-butylpheno...	220	C14H20O2	160875-28-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092923\
Data File : BF135516.D
Acq On : 29 Sep 2023 15:12
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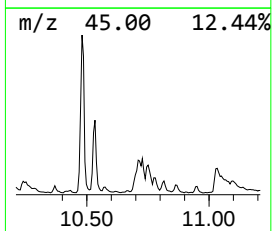
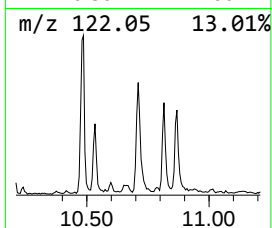
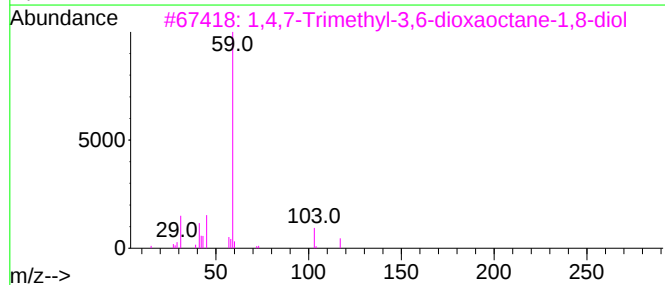
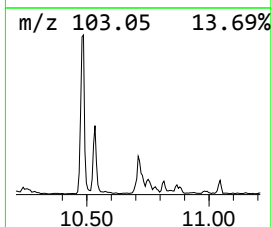
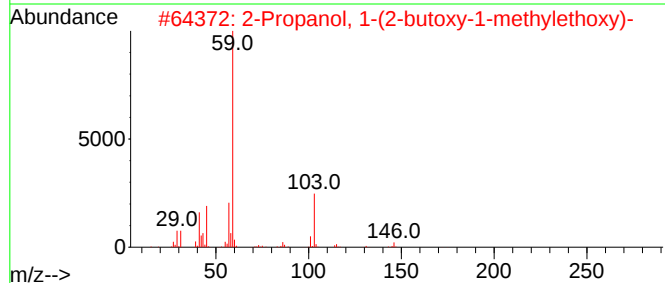
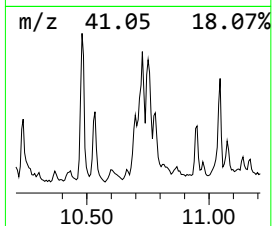
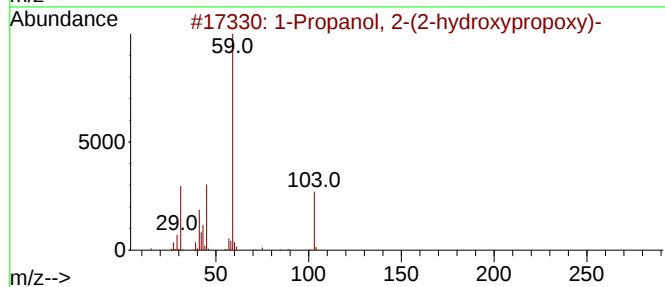
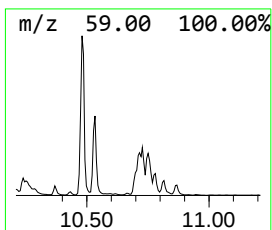
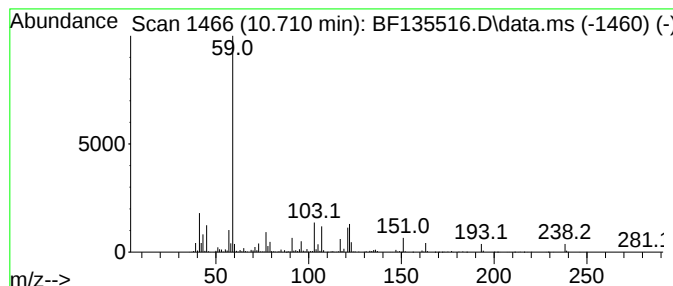
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown10.710 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.710	30.28 ng	1370780	Phenanthrene-d10	11.275

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	47
2		2-Propanol, 1-(2-butoxy-1-methyl...)	190	C10H22O3	029911-28-2	47
3		1,4,7-Trimethyl-3,6-dioxaoctane-...	192	C9H20O4	1000423-63-2	47
4		Pentane, 2-methoxy-	102	C6H14O	006795-88-6	43
5		Pentanamide	101	C5H11NO	000626-97-1	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092923\
Data File : BF135516.D
Acq On : 29 Sep 2023 15:12
Operator : CG\JU
Sample : 04645-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

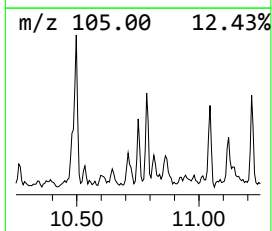
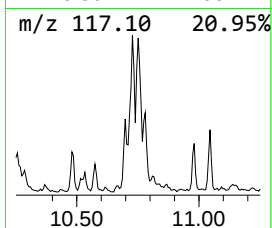
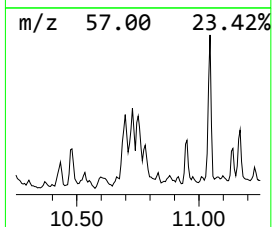
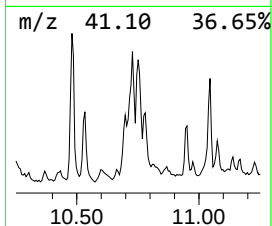
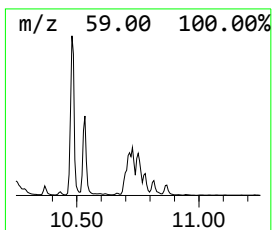
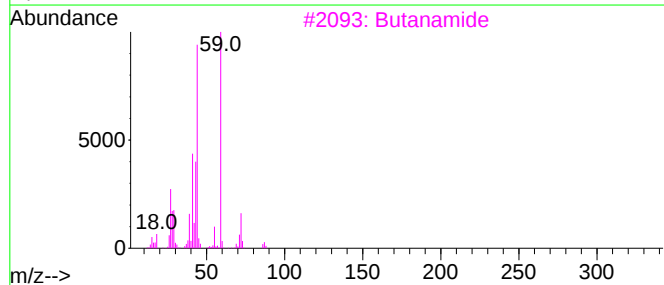
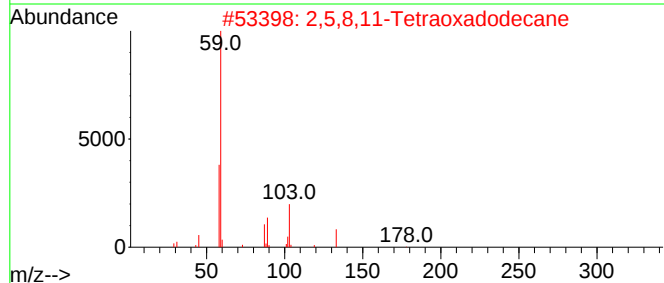
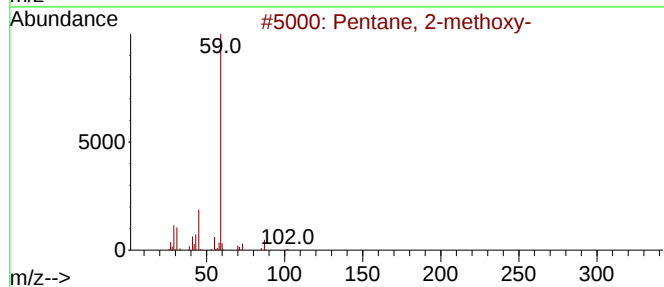
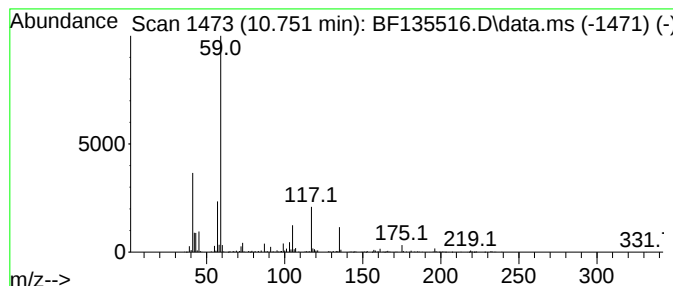
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Pentane, 2-methoxy- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.751	15.05 ng	681524	Phenanthrene-d10		11.275	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Pentane, 2-methoxy-		102	C6H14O	006795-88-6	50
2	2,5,8,11-Tetraoxadodecane		178	C8H18O4	000112-49-2	47
3	Butanamide		87	C4H9NO	000541-35-5	47
4	Tri(propylene glycol) propyl ether		234	C12H26O4	096077-04-2	45
5	4,8,12,16-tetraoxaeicosan-1-ol		306	C16H34O5	1010397-63-6	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092923\
Data File : BF135516.D
Acq On : 29 Sep 2023 15:12
Operator : CG\JU
Sample : 04645-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

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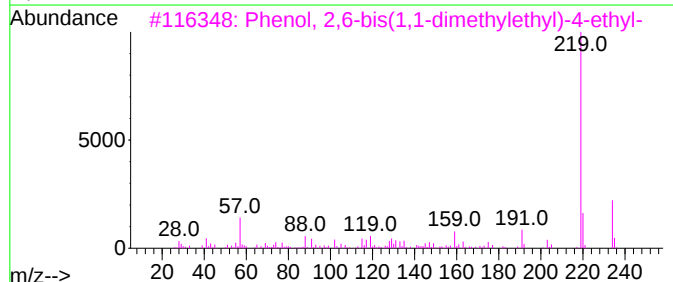
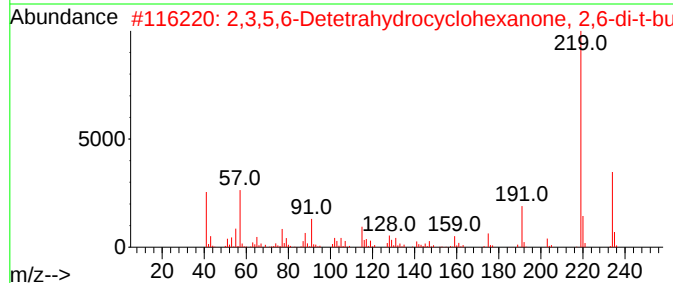
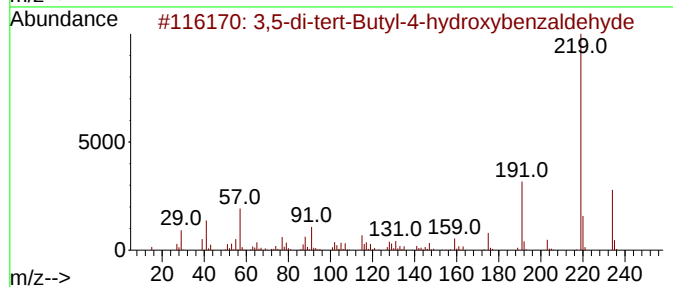
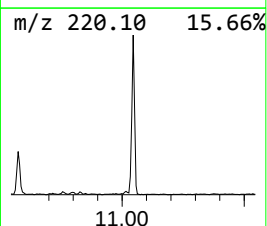
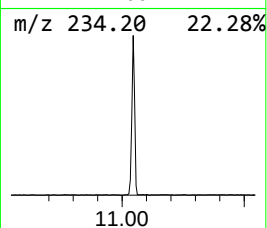
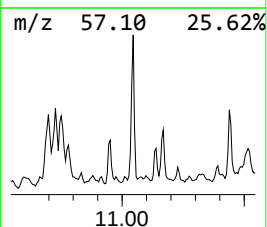
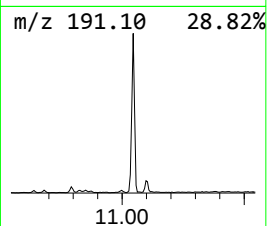
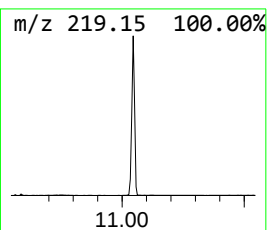
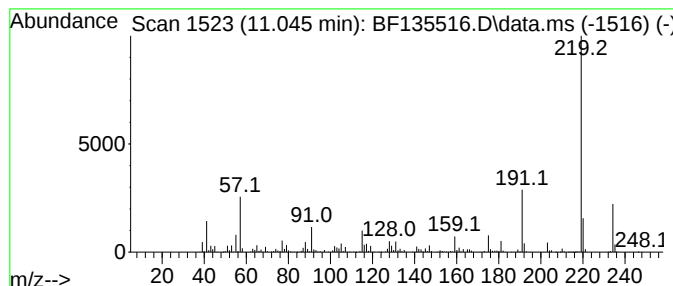
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.045	44.06 ng	1994720	Phenanthrene-d10	11.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	99
2			2,3,5,6-Detetrahydrocyclohexanon...	234	C15H22O2	101100-38-3	95
3			Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	81
4			1-(3-Bromo-2,4-difluorophenyl)et...	234	C8H5BrF2O	1210824-63-7	80
5			4-tert-Butyl-2,6-diisopropylphenol	234	C16H26O	057354-65-1	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092923\
Data File : BF135516.D
Acq On : 29 Sep 2023 15:12
Operator : CG\JU
Sample : 04645-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

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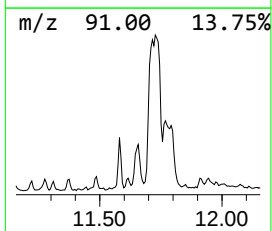
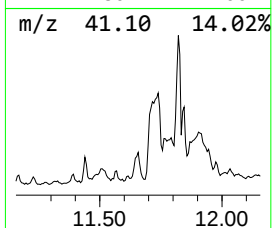
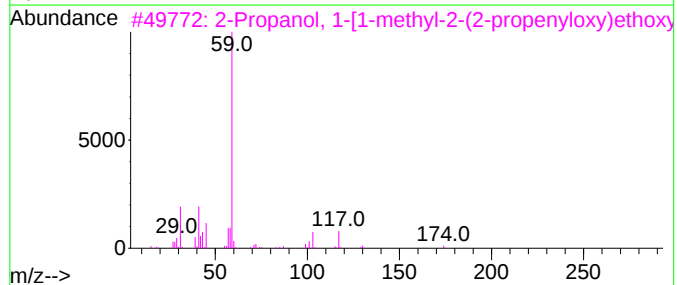
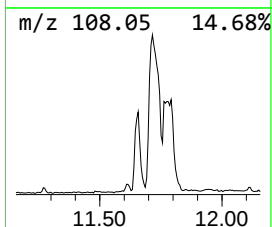
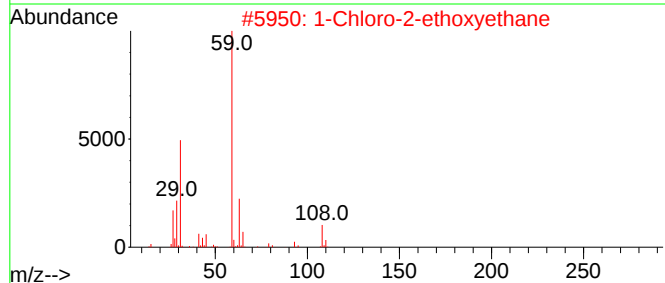
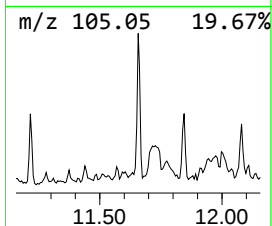
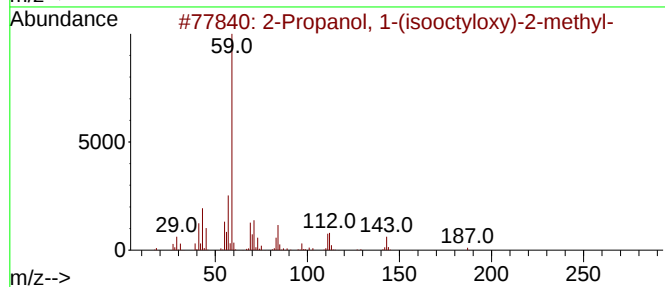
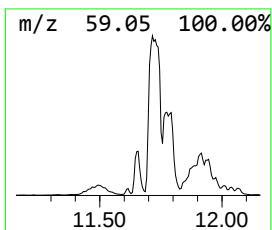
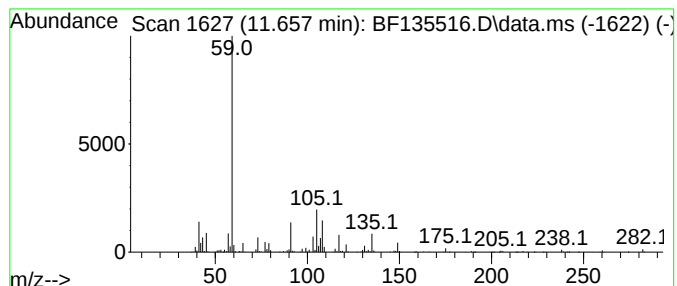
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown11.657 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.657	20.47 ng	926743	Phenanthrene-d10	11.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(isooctyloxy)-2-me...	202	C12H26O2	056282-27-0	43		
2	1-Chloro-2-ethoxyethane	108	C4H9ClO	000628-34-2	40		
3	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	38		
4	1,4,7-Trimethyl-3,6-dioxaoctane-...	192	C9H20O4	1000423-63-2	38		
5	Butanoic acid, 2-hydroxy-, methy...	118	C5H10O3	029674-47-3	37		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092923\
Data File : BF135516.D
Acq On : 29 Sep 2023 15:12
Operator : CG\JU
Sample : 04645-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

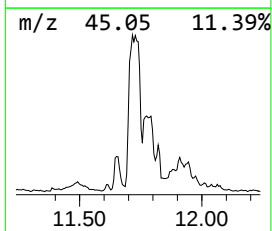
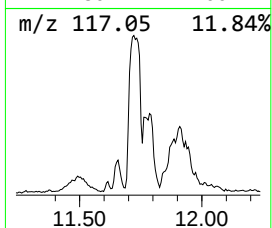
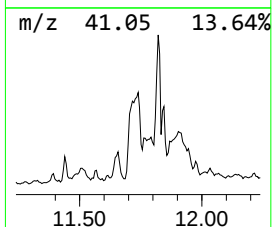
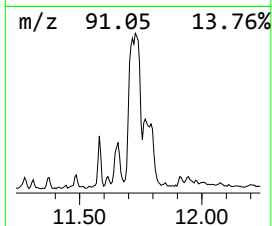
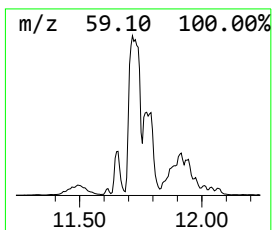
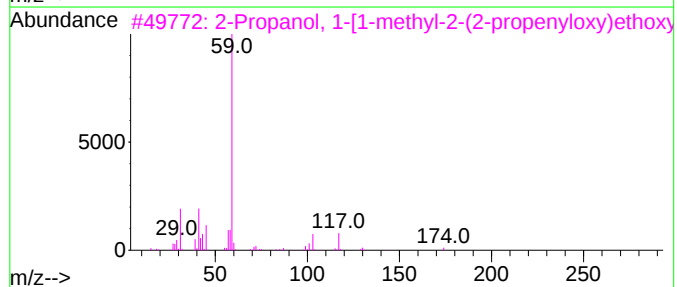
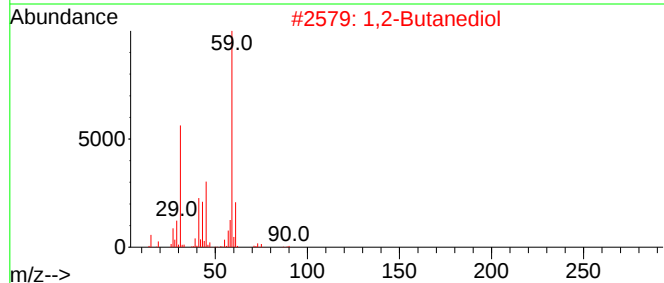
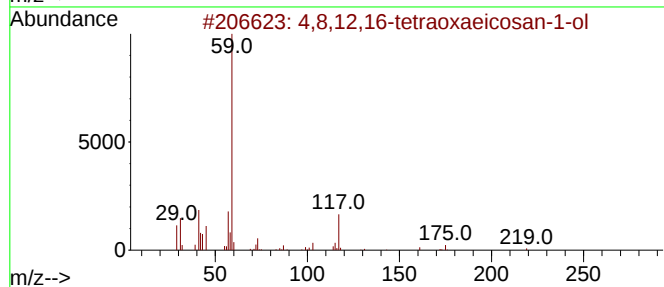
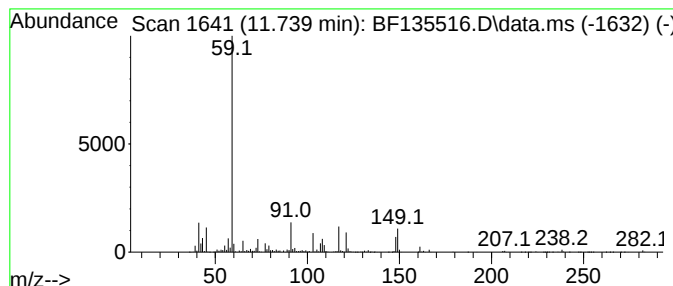
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 4,8,12,16-tetraoxaeicosan-1-ol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.739	159.31 ng	7212350	Phenanthrene-d10	11.275	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,8,12,16-tetraoxaeicosan-1-ol	306	C16H34O5	1010397-63-6	50
2	1,2-Butanediol	90	C4H10O2	000584-03-2	43
3	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	40
4	4,6-Decadiyn-3-ol, 3-isopropyl-9...	296	C17H28O4	1000156-87-6	40
5	Tri(1,2-propyleneglycol), monome...	206	C10H22O4	1000262-26-6	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092923\
Data File : BF135516.D
Acq On : 29 Sep 2023 15:12
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Sample : 04645-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

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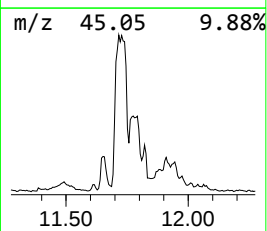
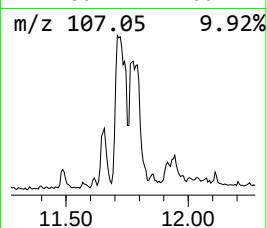
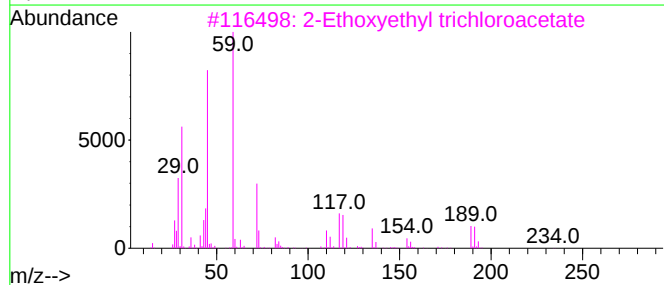
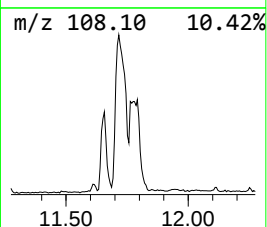
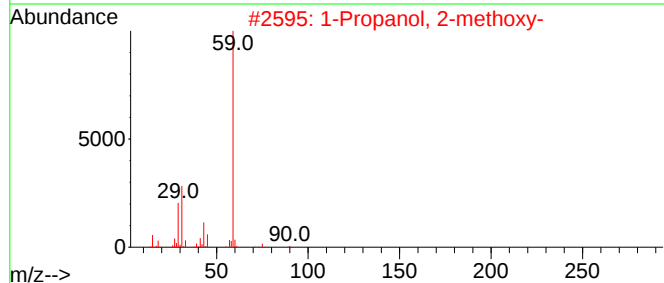
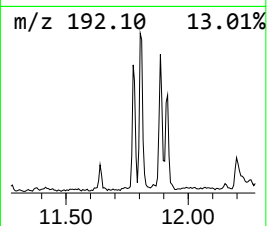
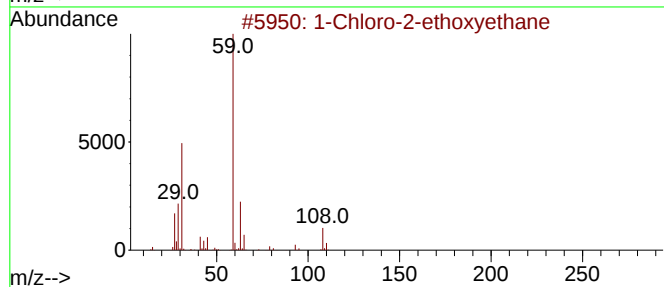
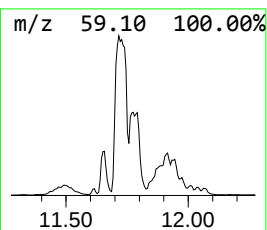
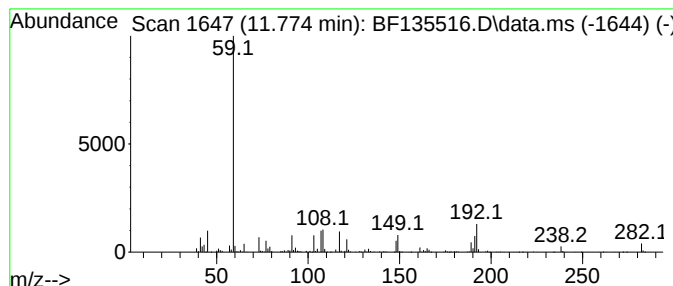
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown11.775 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.775	38.50 ng	1743200	Phenanthrene-d10	11.275

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Chloro-2-ethoxyethane	108	C4H9ClO	000628-34-2	47
2		1-Propanol, 2-methoxy-	90	C4H10O2	001589-47-5	37
3		2-Ethoxyethyl trichloroacetate	234	C6H9Cl3O3	030668-97-4	28
4		2-(2-Methoxyethoxy)propanoic aci...	220	C9H20O4Si	1000506-61-6	28
5		1,2-Benzenediol, 0,0'-di(2-metho...	314	C14H18O8	1000329-80-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092923\
Data File : BF135516.D
Acq On : 29 Sep 2023 15:12
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Sample : 04645-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

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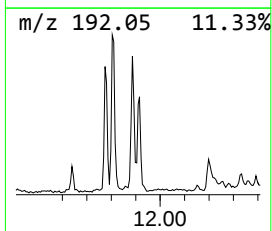
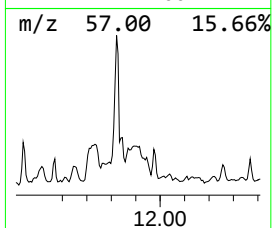
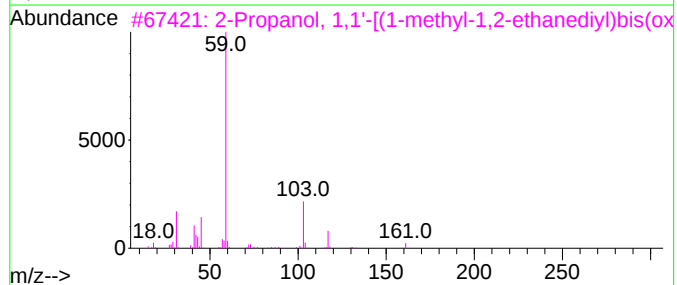
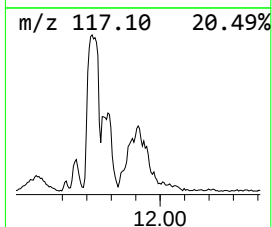
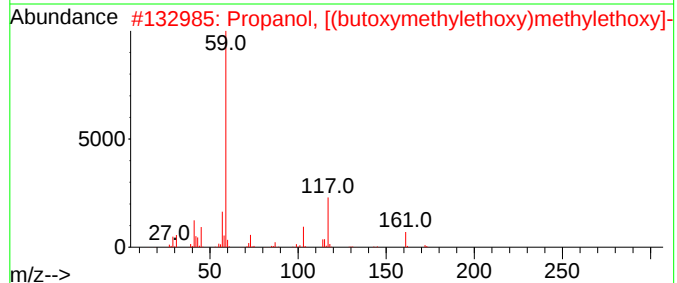
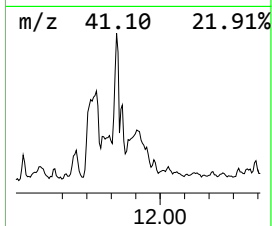
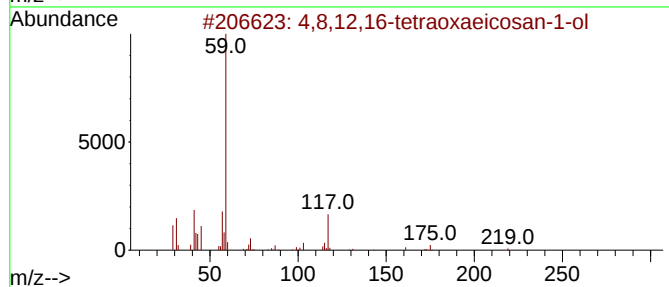
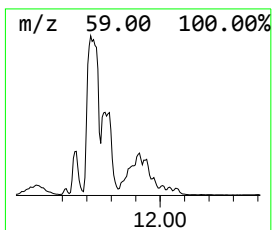
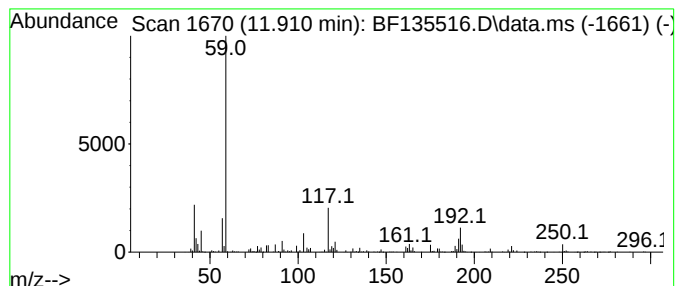
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown11.910 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	19.70 ng	892013	Phenanthrene-d10	11.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,8,12,16-tetraoxaeicosan-1-ol	306	C16H34O5	1010397-63-6	50		
2	Propanol, [(butoxymethylethoxy)m...	248	C13H28O4	055934-93-5	45		
3	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	37		
4	1-(1-Methoxypropan-2-yloxy)propa...	232	C12H24O4	1000367-11-4	28		
5	3,6,9,12,15-Pentaoxahexadecan-1-...	366	C17H38O6Si	1000352-11-8	28		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092923\
Data File : BF135516.D
Acq On : 29 Sep 2023 15:12
Operator : CG\JU
Sample : 04645-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
02

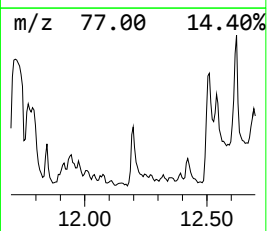
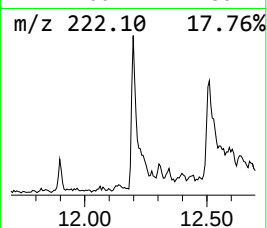
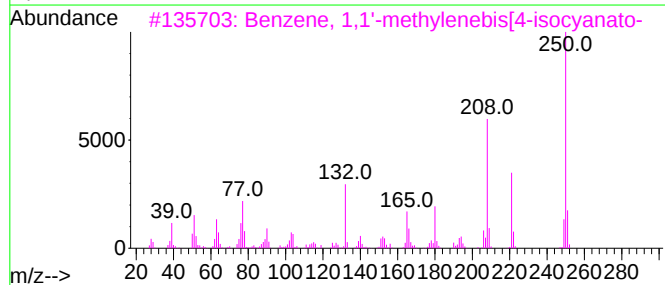
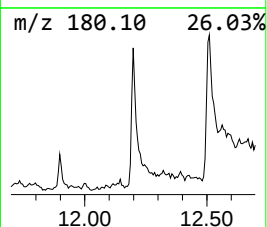
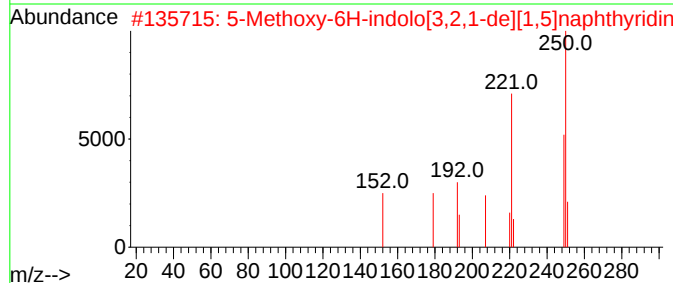
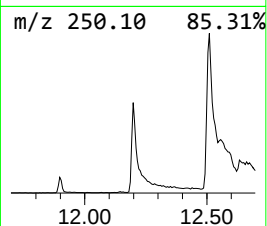
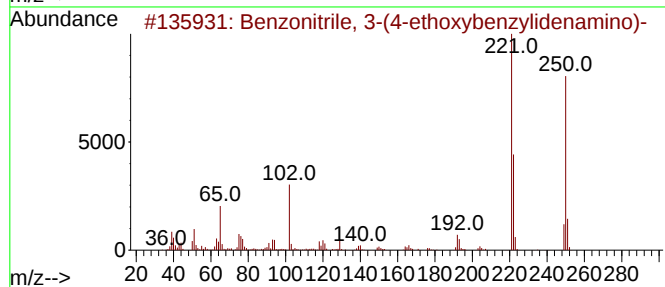
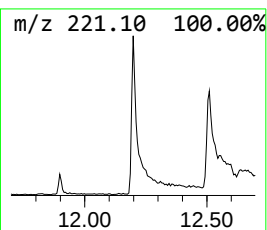
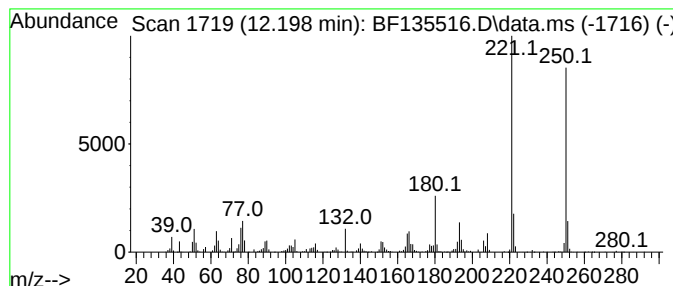
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Benzonitrile, 3-(4-ethoxybe... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.198	23.39 ng	1058770	Phenanthrene-d10	11.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzonitrile, 3-(4-ethoxybenzylid...	250	C16H14N2O	303769-79-1	68
2			5-Methoxy-6H-indolo[3,2,1-de][1,...	250	C15H10N2O2	015071-56-4	50
3			Benzene, 1,1'-methylenebis[4-iso...	250	C15H10N2O2	000101-68-8	49
4			1-Methyl-3,6-diazahomoadamantan-...	250	C12H18N4O2	147084-89-7	38
5			5-Oxo-6-(p-tolyl)-1,2,3,5-tetra...	250	C16H14N2O	1000482-07-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092923\
Data File : BF135516.D
Acq On : 29 Sep 2023 15:12
Operator : CG\JU
Sample : 04645-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

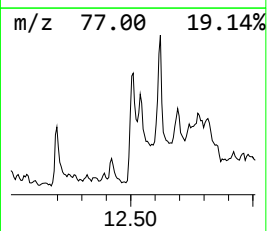
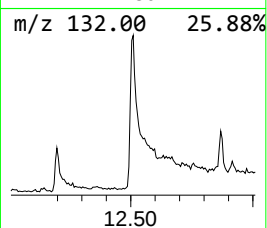
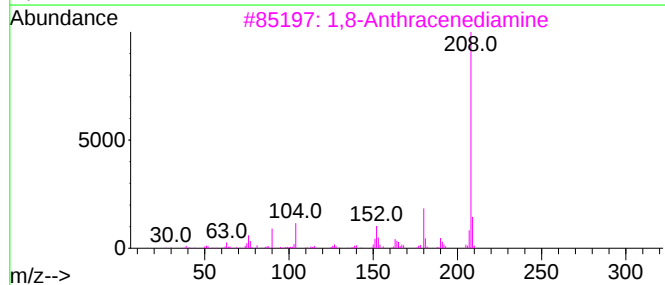
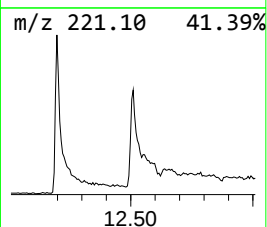
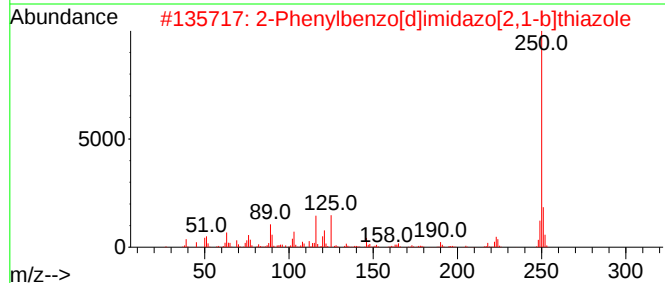
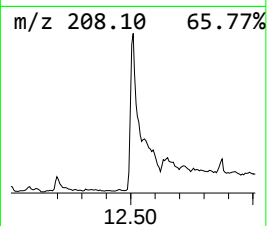
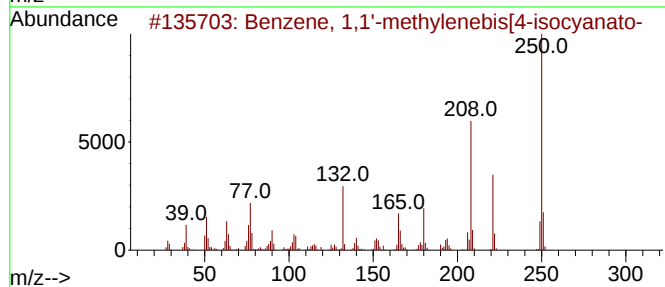
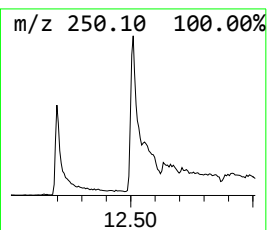
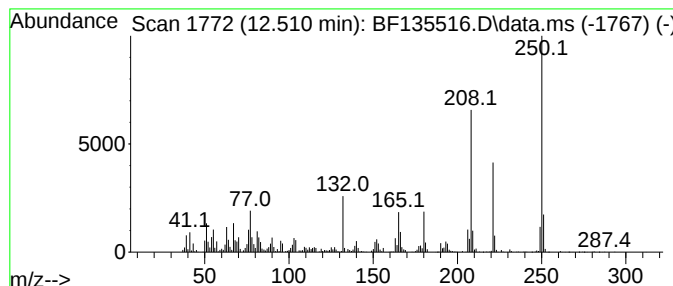
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BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Benzene, 1,1'-methylenebis[... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.510	33.85 ng	1532460	Phenanthrene-d10	11.275	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-methylenebis[4-iso...	250	C15H10N2O2	000101-68-8	99
2	2-Phenylbenzo[d]imidazo[2,1-b]th...	250	C15H10N2S	017833-07-7	38
3	1,8-Anthracenediamine	208	C14H12N2	139312-39-3	25
4	6-Amino-2-(3-methylpiperidin-1-y...	208	C10H16N4O	1000388-66-0	25
5	2-Phenyl-1H-indol-4-amine	208	C14H12N2	500992-25-6	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092923\
Data File : BF135516.D
Acq On : 29 Sep 2023 15:12
Operator : CG\JU
Sample : 04645-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
02

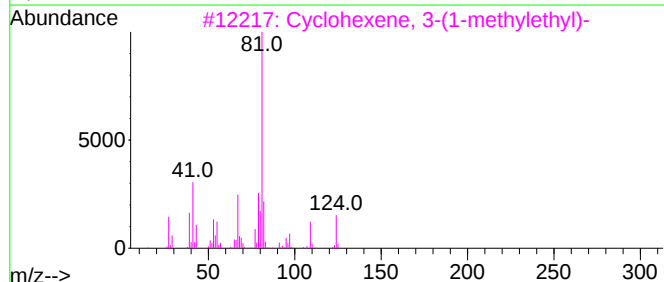
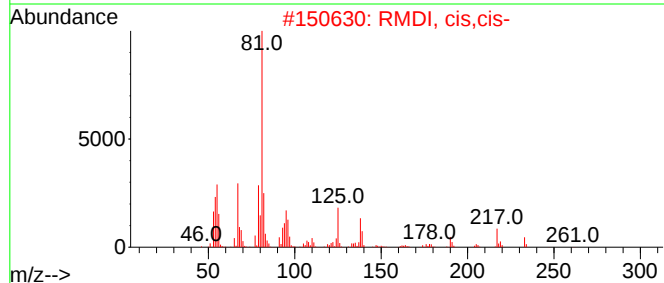
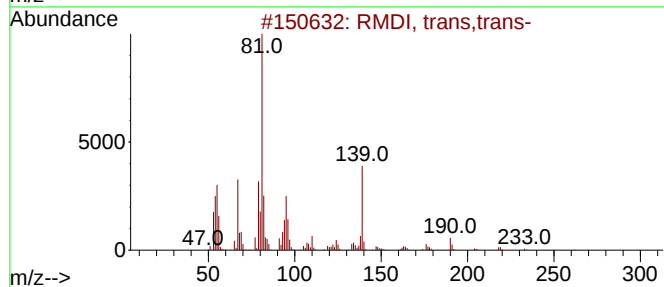
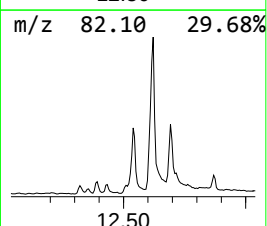
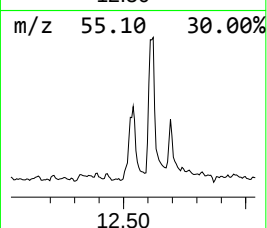
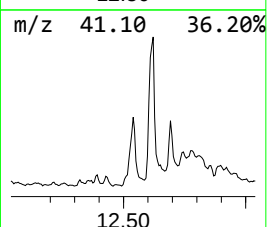
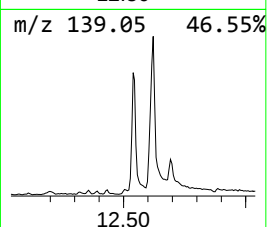
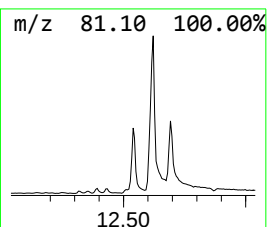
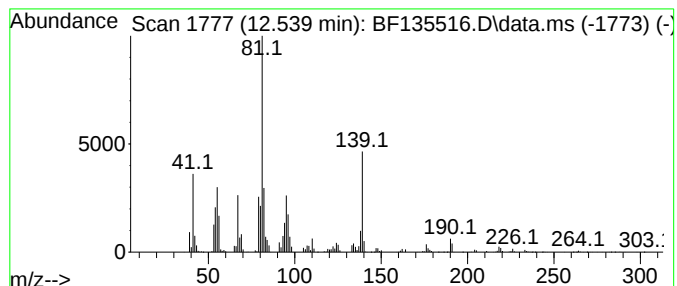
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 RMDI, trans,trans- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.539	65.28 ng	2955340	Phenanthrene-d10	11.275

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		RMDI, trans,trans-	262	C15H22N2O2	013622-90-7	97
2		RMDI, cis,cis-	262	C15H22N2O2	018937-00-3	86
3		Cyclohexene, 3-(1-methylethyl)-	124	C9H16	003983-08-2	50
4		Cyclohexene, 1-butyl-	138	C10H18	003282-53-9	47
5		RMDI, Cis,trans-	262	C15H22N2O2	017901-48-3	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092923\
Data File : BF135516.D
Acq On : 29 Sep 2023 15:12
Operator : CG\JU
Sample : 04645-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

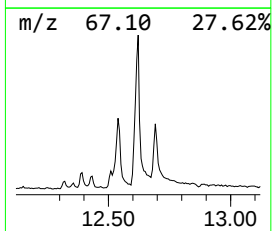
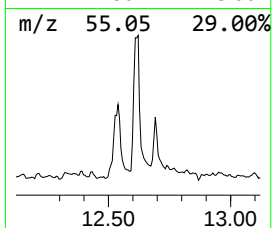
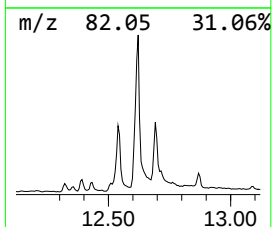
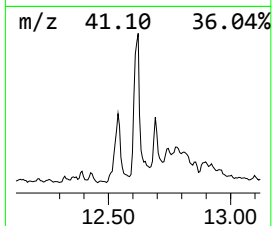
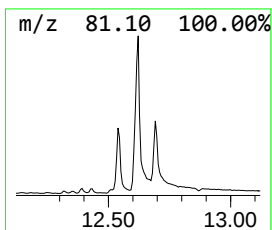
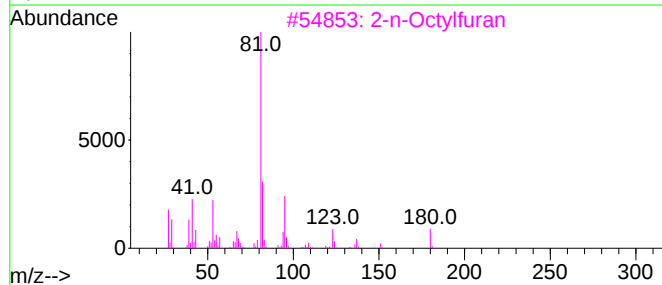
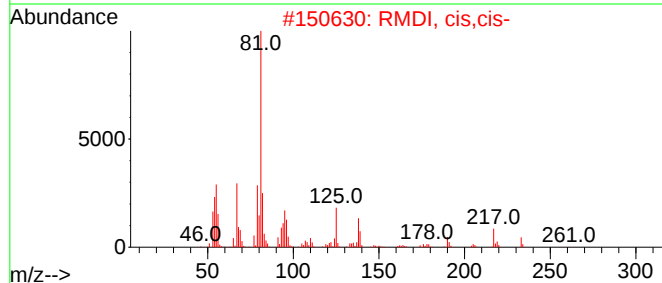
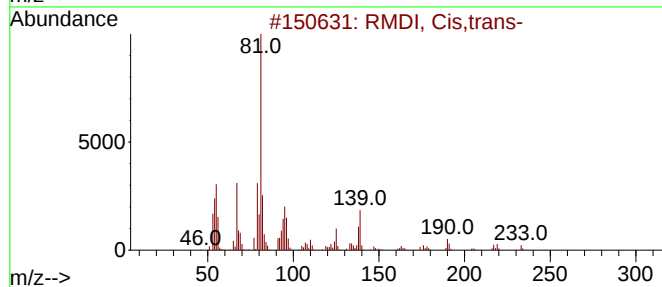
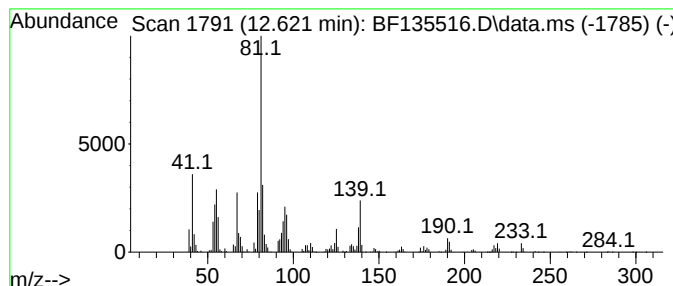
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 RMDI, Cis,trans- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.621	27.54 ng	7676400	Chrysene-d12		13.933	
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		RMDI, Cis,trans-	262	C15H22N2O2	017901-48-3	91
2		RMDI, cis,cis-	262	C15H22N2O2	018937-00-3	74
3		2-n-Octylfuran	180	C12H20O	004179-38-8	50
4		Cyclohexene,3-butyl-	138	C10H18	003983-07-1	50
5		2,4-Nonadienal, (E,E)-	138	C9H14O	005910-87-2	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092923\
Data File : BF135516.D
Acq On : 29 Sep 2023 15:12
Operator : CG\JU
Sample : 04645-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(S)-(+)-1,2-Pro...	3.375	77.7	ng	3815730	1	6.745	981634	20.0
unknown7.722	7.722	15.9	ng	849454	2	8.022	1065680	20.0
1,3-Pentanediol...	7.739	18.6	ng	992320	2	8.022	1065680	20.0
unknown8.286	8.286	15.0	ng	800151	2	8.022	1065680	20.0
1-Propanol, 2-(...	8.675	17.5	ng	934337	2	8.022	1065680	20.0
1-Propanol, 2,2...	8.704	37.7	ng	2009970	2	8.022	1065680	20.0
Tri(propylene g...	8.781	18.1	ng	967290	2	8.022	1065680	20.0
2,6-Di-tert-but...	9.533	20.4	ng	1269690	3	9.780	1244530	20.0
2,5-Cyclohexadi...	9.598	20.6	ng	1282030	3	9.780	1244530	20.0
unknown10.710	10.710	30.3	ng	1370780	4	11.275	905445	20.0
Pentane, 2-meth...	10.751	15.1	ng	681524	4	11.275	905445	20.0
3,5-di-tert-But...	11.045	44.1	ng	1994720	4	11.275	905445	20.0
unknown11.657	11.657	20.5	ng	926743	4	11.275	905445	20.0
4,8,12,16-tetra...	11.739	159.3	ng	7212350	4	11.275	905445	20.0
unknown11.775	11.775	38.5	ng	1743200	4	11.275	905445	20.0
unknown11.910	11.910	19.7	ng	892013	4	11.275	905445	20.0
Benzonitrile, 3...	12.198	23.4	ng	1058770	4	11.275	905445	20.0
Benzene, 1,1'-m...	12.510	33.9	ng	1532460	4	11.275	905445	20.0
RMDI, trans,trans-	12.539	65.3	ng	2955340	4	11.275	905445	20.0
RMDI, Cis,trans-	12.621	27.5	ng	7676400	5	13.933	5573740	20.0