

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
 Data File : BF133811.D
 Acq On : 16 Jun 2023 17:30
 Operator : CG\JU
 Sample : 03222-19 2X
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSIT-SB-16

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-BF060923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133811.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	21	rVB	199493	286288	27.33%	1.447%
2	3.957	313	318	323	rVB	95201	120491	11.50%	0.609%
3	5.087	506	510	518	rVB	59319	64055	6.11%	0.324%
4	5.357	552	556	560	rBV	319462	295115	28.17%	1.492%
5	5.463	570	574	575	rBV	41412	42216	4.03%	0.213%
6	5.487	575	578	590	rVB	993875	864484	82.53%	4.370%
7	5.710	612	616	625	rVB	815805	758758	72.43%	3.835%
8	6.040	668	672	675	rBV	50578	43450	4.15%	0.220%
9	6.328	718	721	726	rVB	25807	20871	1.99%	0.105%
10	6.392	729	732	734	rBV	24098	21161	2.02%	0.107%
11	6.487	745	748	754	rBV	920410	784624	74.90%	3.966%
12	6.687	780	782	786	rBV2	33567	37876	3.62%	0.191%
13	6.863	808	812	816	rBV	619505	488600	46.64%	2.470%
14	7.145	856	860	862	rVB	55787	47731	4.56%	0.241%
15	7.257	875	879	884	rBV5	9892	16534	1.58%	0.084%
16	7.422	903	907	911	rBV	570775	492039	46.97%	2.487%
17	7.451	911	912	916	rVB	27039	20377	1.95%	0.103%
18	7.886	983	986	991	rVB3	13194	18049	1.72%	0.091%
19	8.139	1026	1029	1031	rBV	737340	612788	58.50%	3.098%
20	8.163	1031	1033	1037	rVB	299218	217155	20.73%	1.098%
21	8.416	1073	1076	1078	rBV	43198	34660	3.31%	0.175%
22	8.728	1126	1129	1134	rBV2	39842	36829	3.52%	0.186%
23	8.851	1147	1150	1153	rBV	143969	114874	10.97%	0.581%
24	8.951	1164	1167	1170	rBV	119292	90789	8.67%	0.459%
25	9.216	1208	1212	1215	rBV	1410367	1047515	100.00%	5.295%
26	9.298	1220	1226	1227	rVV	32036	30828	2.94%	0.156%
27	9.316	1227	1229	1235	rVB	44268	39590	3.78%	0.200%
28	9.422	1243	1247	1249	rBV2	52750	53292	5.09%	0.269%
29	9.475	1252	1256	1262	rVB4	25070	44684	4.27%	0.226%
30	9.551	1267	1269	1272	rBV	33985	35080	3.35%	0.177%
31	9.580	1272	1274	1276	rVV	21230	16342	1.56%	0.083%
32	9.610	1276	1279	1282	rVV2	33325	36497	3.48%	0.184%
33	9.710	1294	1296	1299	rVB4	21313	17553	1.68%	0.089%
34	9.757	1301	1304	1306	rBV	40563	34024	3.25%	0.172%
35	9.780	1306	1308	1311	rVV	22983	20892	1.99%	0.106%
36	9.828	1314	1316	1319	rVB	28239	18366	1.75%	0.093%

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Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	9.898	1324	1328	1331	rVV	944491	745818	71.20%	3.770%
38	9.928	1331	1333	1337	rVB2	43465	40289	3.85%	0.204%
39	10.051	1349	1354	1358	rBV8	10122	18189	1.74%	0.092%
40	10.104	1358	1363	1367	rVV2	51198	63903	6.10%	0.323%
41	10.139	1367	1369	1374	rVB5	16141	23178	2.21%	0.117%
42	10.327	1399	1401	1404	rVB3	25276	19832	1.89%	0.100%
43	10.410	1411	1415	1418	rVB6	12497	16786	1.60%	0.085%
44	10.445	1418	1421	1427	rBV2	55343	57122	5.45%	0.289%
45	10.610	1446	1449	1453	rVB	230799	196663	18.77%	0.994%
46	10.686	1458	1462	1466	rVV	698206	584831	55.83%	2.956%
47	10.739	1469	1471	1477	rVB3	24097	25817	2.46%	0.131%
48	10.804	1479	1482	1487	rBV4	49824	70575	6.74%	0.357%
49	10.933	1494	1504	1509	rBV7	51973	102419	9.78%	0.518%
50	10.992	1510	1514	1517	rVV	314110	255003	24.34%	1.289%
51	11.133	1535	1538	1540	rBV3	18017	20484	1.96%	0.104%
52	11.163	1540	1543	1546	rVB2	42445	38001	3.63%	0.192%
53	11.192	1546	1548	1551	rBV	48687	48052	4.59%	0.243%
54	11.251	1556	1558	1561	rVV3	36330	34351	3.28%	0.174%
55	11.286	1561	1564	1567	rVB	40186	34844	3.33%	0.176%
56	11.351	1572	1575	1577	rBV3	21554	17913	1.71%	0.091%
57	11.392	1578	1582	1584	rVV	754781	664262	63.41%	3.358%
58	11.416	1584	1586	1589	rVV	403326	317160	30.28%	1.603%
59	11.463	1592	1594	1597	rVV	116392	108827	10.39%	0.550%
60	11.498	1597	1600	1604	rVB2	35756	36573	3.49%	0.185%
61	11.622	1619	1621	1624	rBV	34204	31115	2.97%	0.157%
62	11.686	1629	1632	1634	rVB3	31580	25625	2.45%	0.130%
63	11.722	1635	1638	1643	rVV5	35493	44527	4.25%	0.225%
64	11.769	1643	1646	1647	rVV2	30682	32502	3.10%	0.164%
65	11.786	1647	1649	1651	rVV	89292	67367	6.43%	0.341%
66	11.810	1651	1653	1656	rVB	36155	29411	2.81%	0.149%
67	11.892	1663	1667	1669	rBV2	78149	99753	9.52%	0.504%
68	11.921	1669	1672	1682	rVV2	546221	630027	60.14%	3.185%
69	11.998	1682	1685	1689	rVV2	339377	343848	32.83%	1.738%
70	12.057	1692	1695	1697	rVV	327736	310430	29.63%	1.569%
71	12.086	1697	1700	1705	rVV	506692	600528	57.33%	3.036%
72	12.151	1709	1711	1713	rVV	76153	73578	7.02%	0.372%
73	12.174	1713	1715	1717	rVV2	58126	59405	5.67%	0.300%
74	12.216	1720	1722	1728	rVB5	52653	92731	8.85%	0.469%
75	12.416	1753	1756	1759	rVB	171443	145609	13.90%	0.736%
76	12.451	1759	1762	1764	rBV	56218	57864	5.52%	0.292%

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77	12.504	1768	1771	1775	rVB	189482	187923	17.94%	0.950%
78	12.610	1786	1789	1791	rBV	612960	522015	49.83%	2.639%
79	12.633	1791	1793	1795	rVV2	98472	85873	8.20%	0.434%
80	12.710	1803	1806	1813	rBV4	73810	102280	9.76%	0.517%
81	12.845	1823	1829	1831	rBV	489652	542210	51.76%	2.741%
82	12.892	1835	1837	1844	rVB2	180706	201617	19.25%	1.019%
83	12.957	1846	1848	1849	rBV	36454	28543	2.72%	0.144%
84	12.986	1849	1853	1858	rVB	972650	810464	77.37%	4.097%
85	13.098	1869	1872	1874	rBV	215389	177341	16.93%	0.896%
86	13.121	1874	1876	1879	rVB	117599	96894	9.25%	0.490%
87	13.174	1881	1885	1891	rVV3	271809	458907	43.81%	2.320%
88	13.233	1891	1895	1898	rVV3	149621	189760	18.12%	0.959%
89	13.404	1921	1924	1927	rBV3	57451	67299	6.42%	0.340%
90	13.468	1932	1935	1938	rBV	261842	271083	25.88%	1.370%
91	13.686	1969	1972	1976	rVB2	103156	122301	11.68%	0.618%
92	13.845	1997	1999	2005	rBV4	99085	118985	11.36%	0.601%
93	14.033	2027	2031	2033	rBV2	757334	918155	87.65%	4.641%
94	14.074	2036	2038	2040	rVB	206904	156269	14.92%	0.790%
95	14.257	2065	2069	2071	rBV	373077	378783	36.16%	1.915%
96	14.410	2093	2095	2098	rVB	145818	131246	12.53%	0.663%
97	15.115	2211	2215	2218	rBV	162967	278205	26.56%	1.406%
98	15.492	2276	2279	2286	rVB	121768	219707	20.97%	1.111%
99	15.562	2287	2291	2294	rBV	214177	278727	26.61%	1.409%
100	16.309	2414	2418	2433	rVB5	124913	328747	31.38%	1.662%

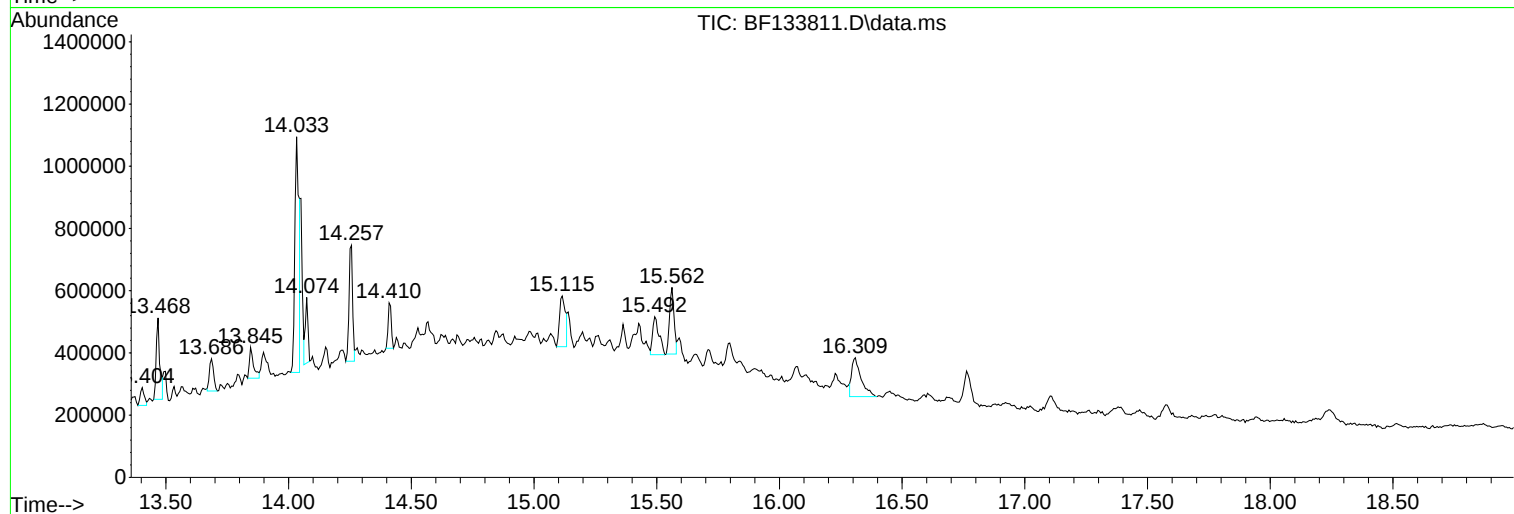
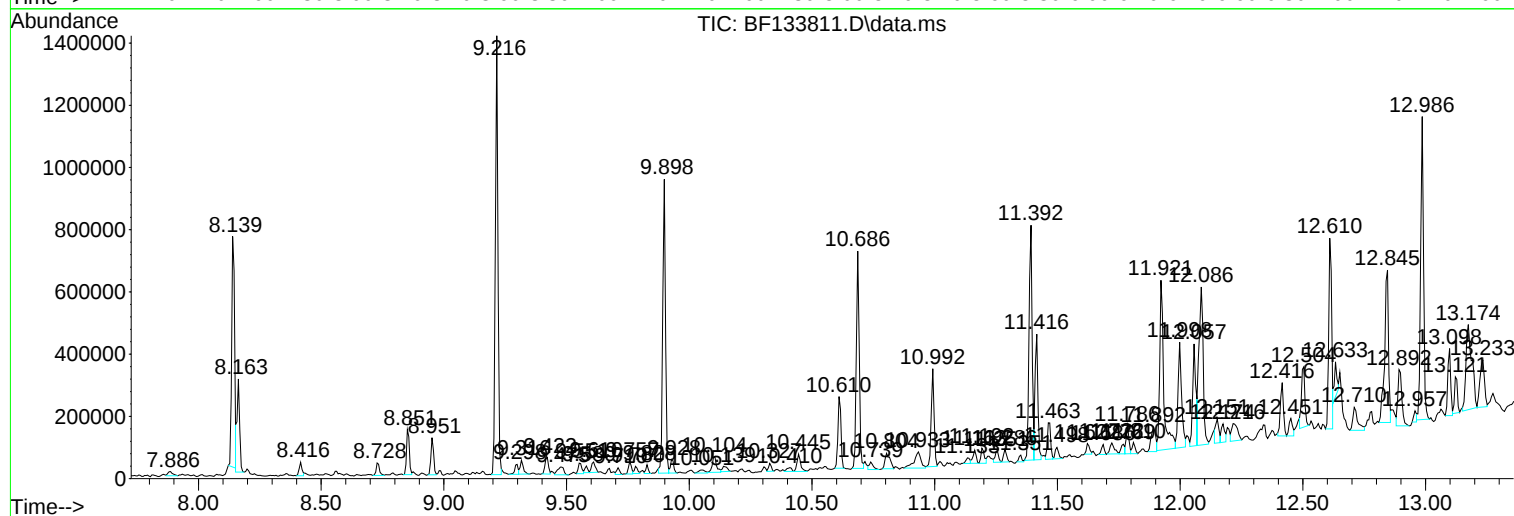
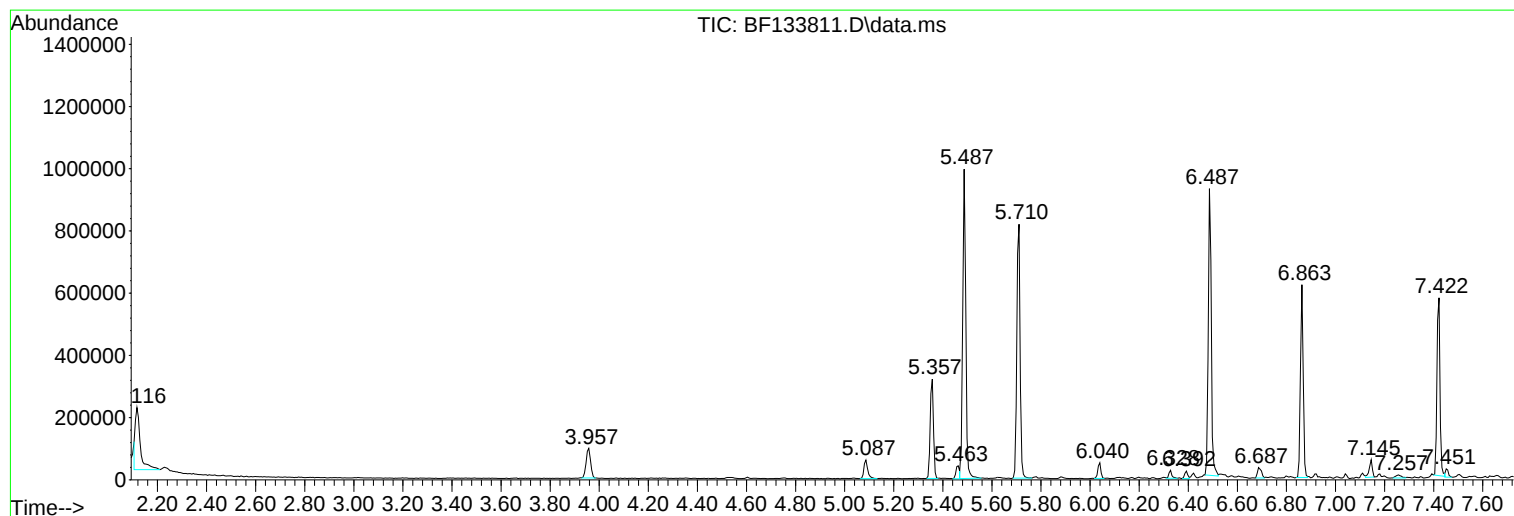
Sum of corrected areas: 19783023

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ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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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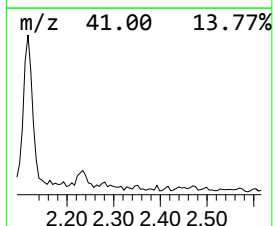
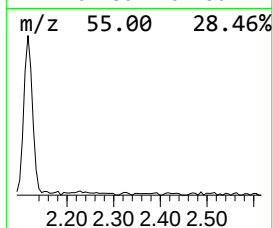
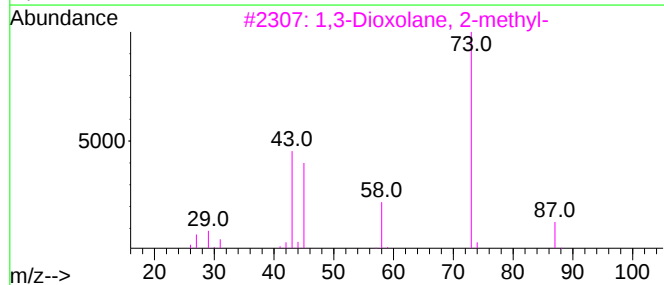
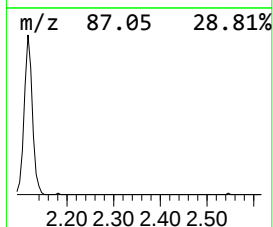
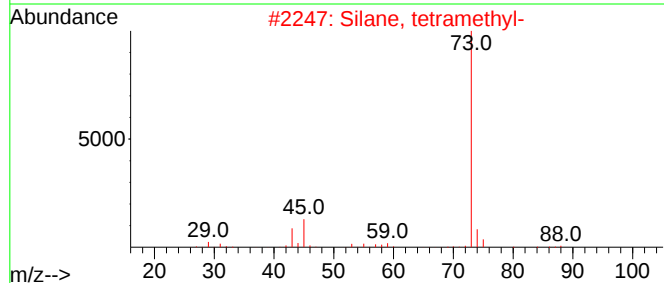
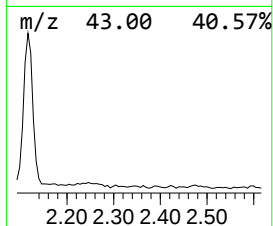
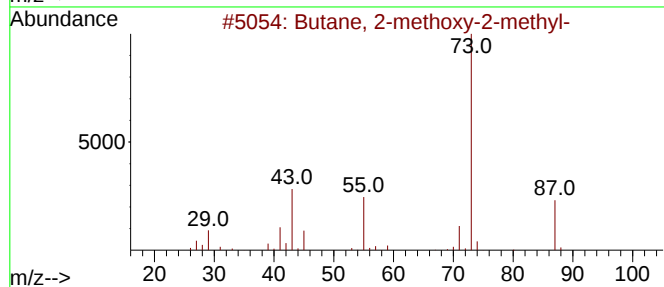
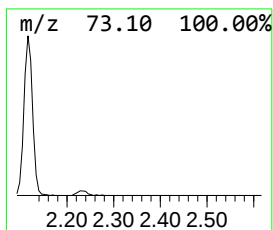
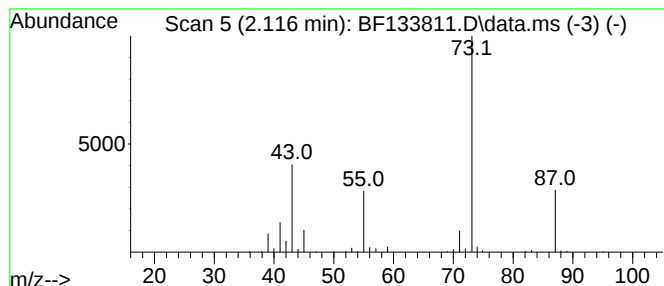
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	11.72 ng	286288	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	56
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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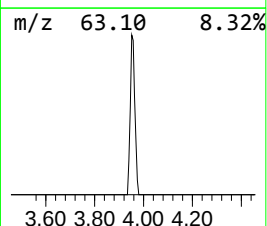
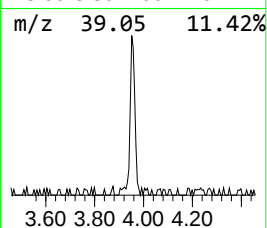
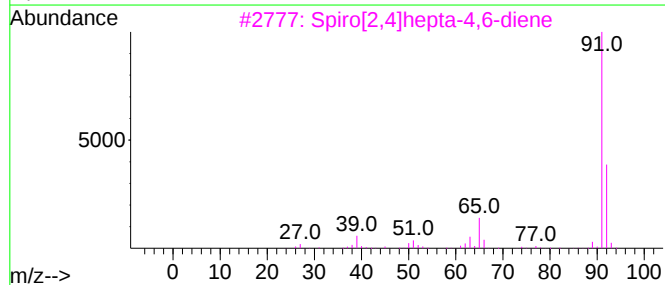
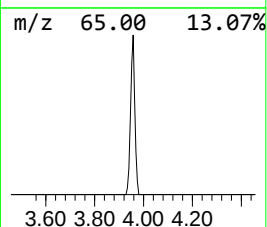
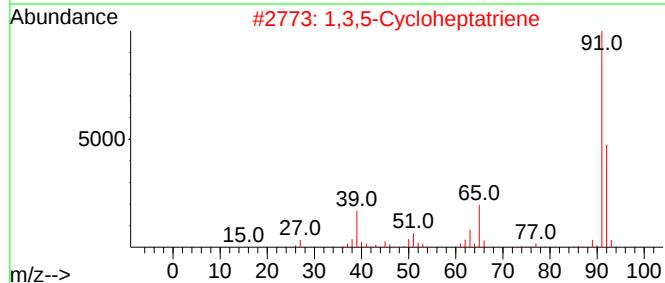
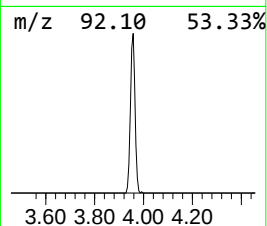
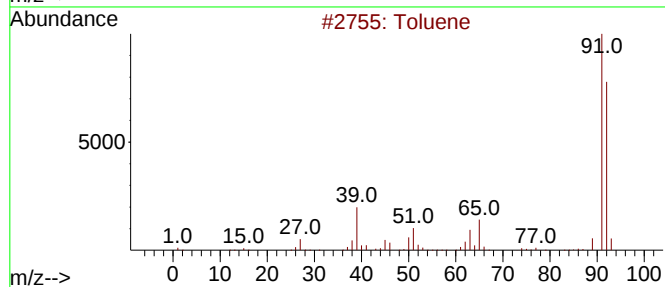
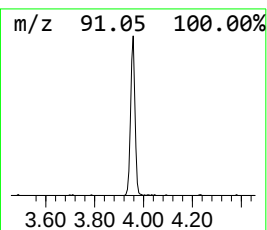
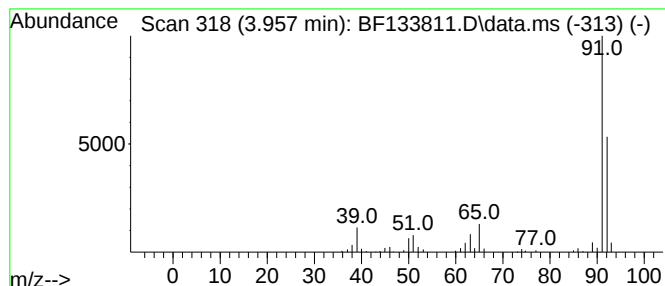
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1,3,5-Cycloheptatriene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.957	4.93 ng	120491	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Toluene	92	C7H8	000108-88-3	95
2			1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	87
3			Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	87
4			2,5-Norbornadiene	92	C7H8	000121-46-0	83
5			Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	59



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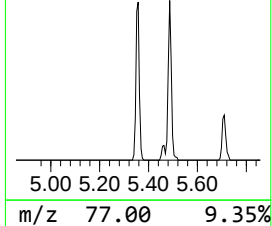
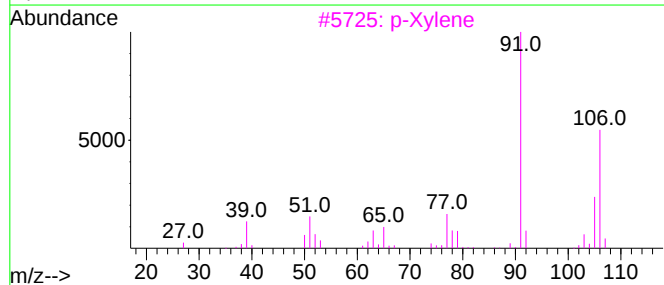
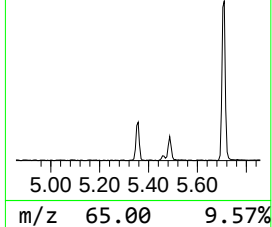
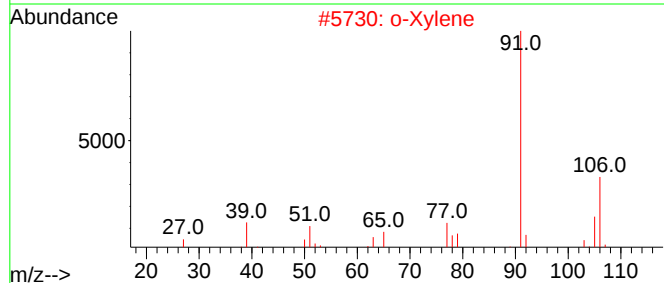
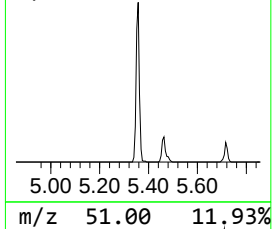
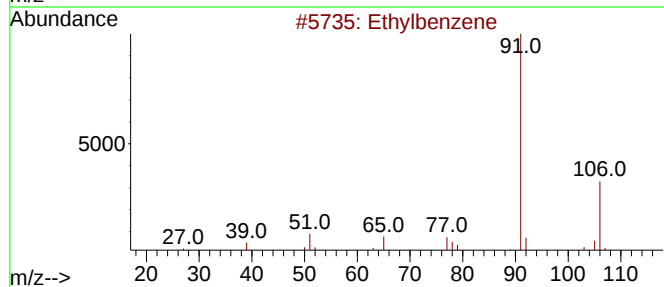
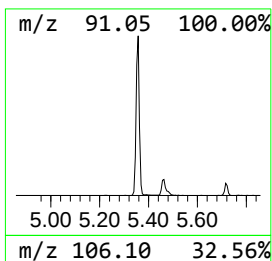
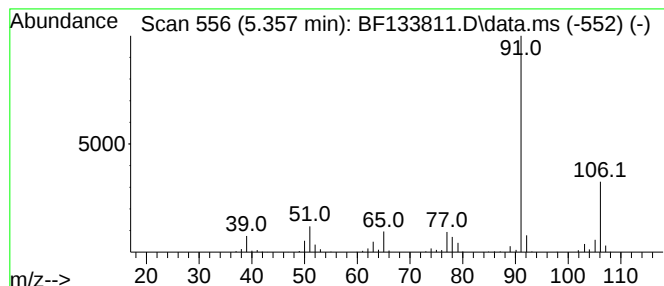
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Ethylbenzene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.357	12.08 ng	295115	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethylbenzene	106	C8H10	000100-41-4	94
2			o-Xylene	106	C8H10	000095-47-6	91
3			p-Xylene	106	C8H10	000106-42-3	81
4			Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	76
5			1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	72



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Data File : BF133811.D
Acq On : 16 Jun 2023 17:30
Operator : CG\JU
Sample : 03222-19 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

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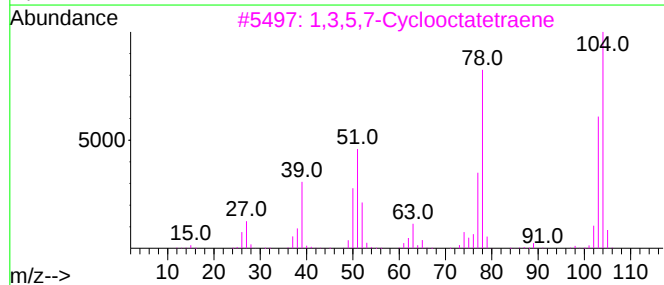
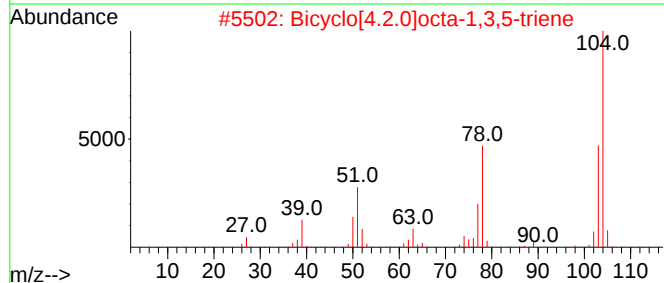
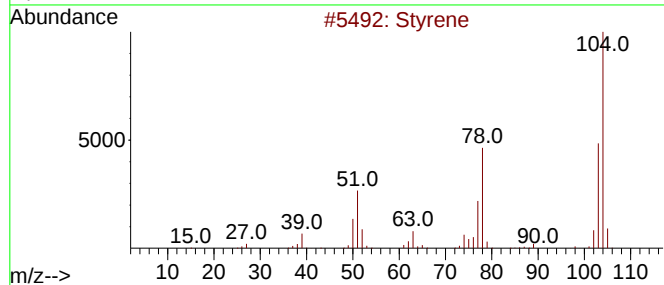
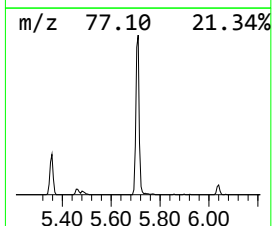
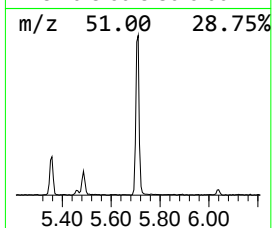
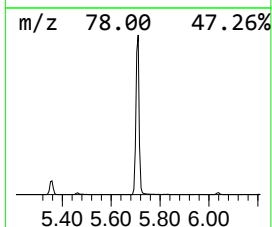
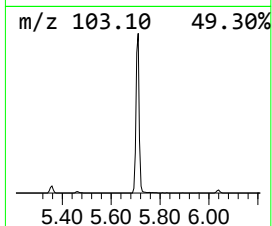
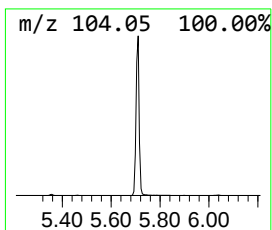
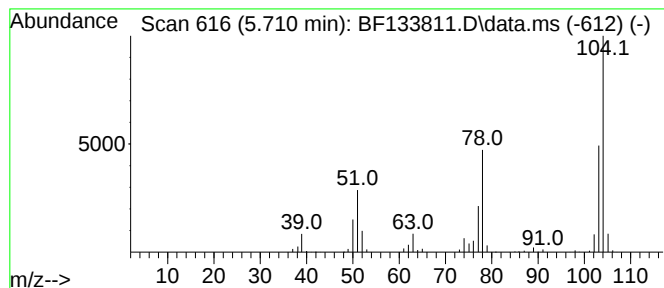
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Styrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.710	31.06 ng	758758	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Styrene	104	C8H8	000100-42-5	96
2			Bicyclo[4.2.0]octa-1,3,5-triene	104	C8H8	000694-87-1	96
3			1,3,5,7-Cyclooctatetraene	104	C8H8	000629-20-9	91
4			Benzene, 1,1'-(1,2-cyclobutanedi...	208	C16H16	007694-30-6	64
5			2-Pyridinecarbonitrile	104	C6H4N2	000100-70-9	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
Data File : BF133811.D
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ClientSampleId :
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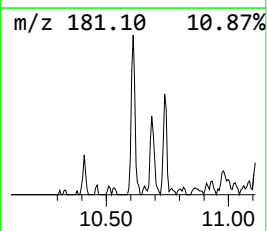
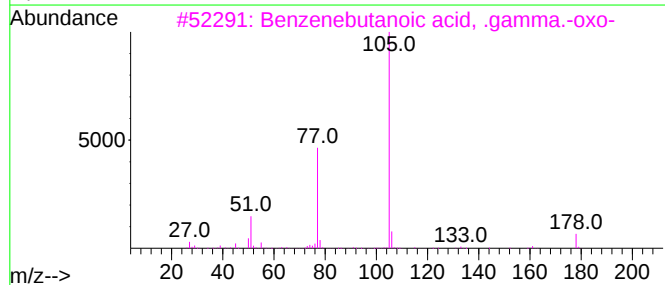
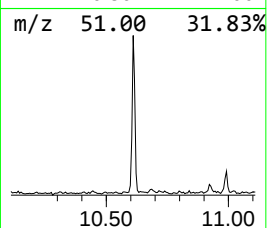
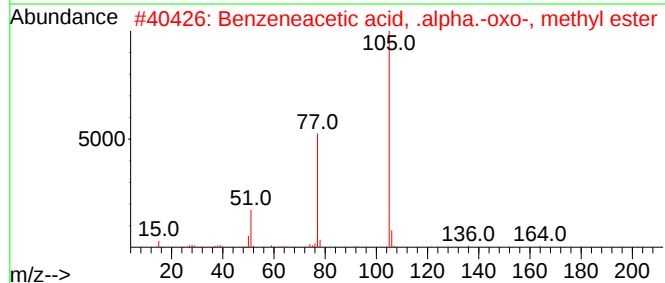
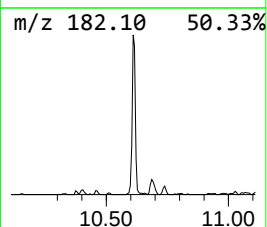
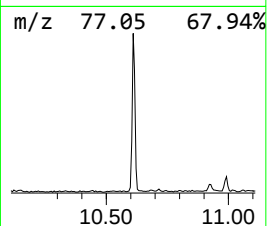
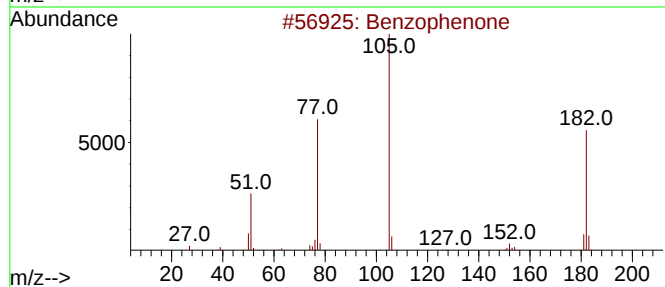
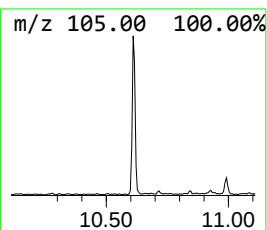
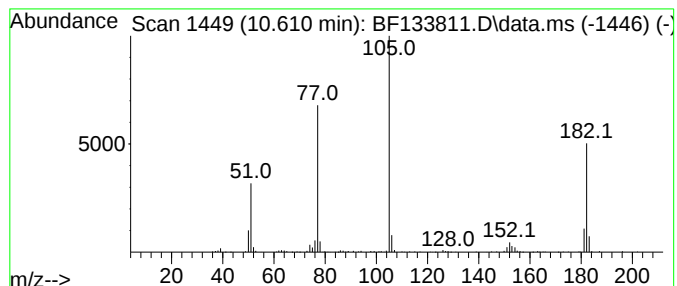
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzophenone Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.610	5.27 ng	196663	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	49
3			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
5			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
Data File : BF133811.D
Acq On : 16 Jun 2023 17:30
Operator : CG\JU
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Misc :
ALS Vial : 9 Sample Multiplier: 1

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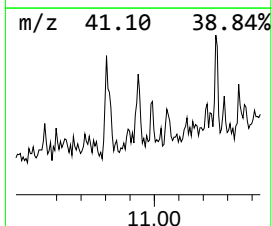
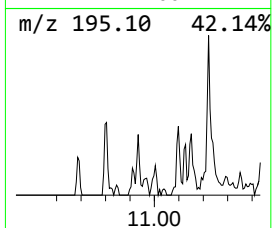
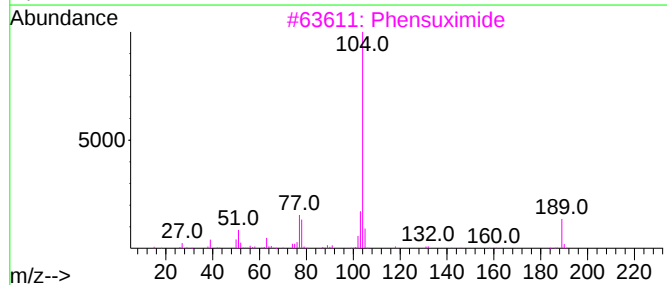
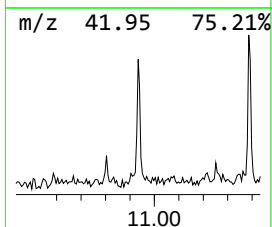
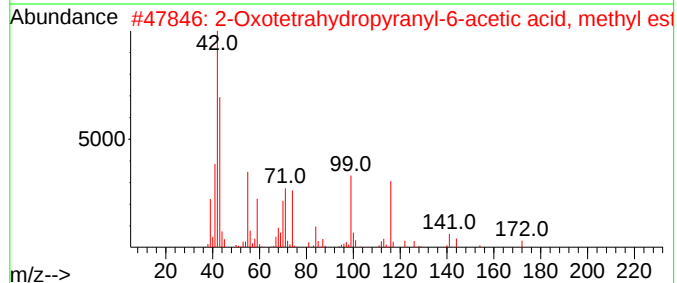
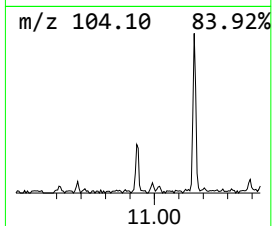
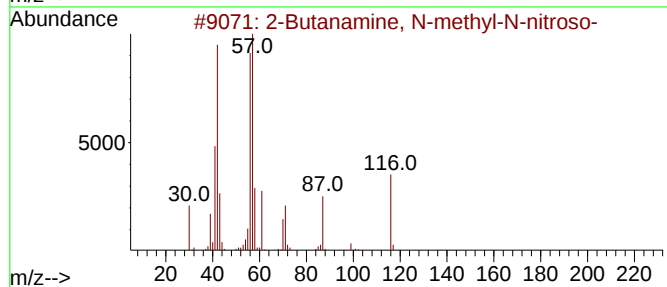
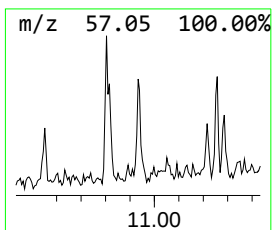
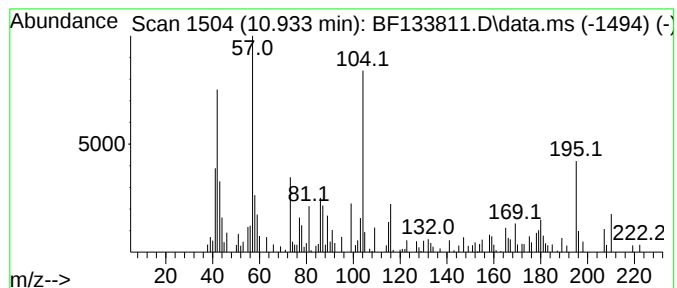
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown10.933 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.933	3.08 ng	102419	Phenanthrene-d10	11.392

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Butanamine, N-methyl-N-nitroso-	116	C5H12N2O	035606-37-2	27
2		2-Oxotetrahydropyranyl-6-acetic ...	172	C8H12O4	1000153-52-7	22
3		Phensuximide	189	C11H11NO2	000086-34-0	15
4		2-Methylbenzyl cyanide	131	C9H9N	022364-68-7	14
5		Cyclobutane, 1,2-diphenyl-	208	C16H16	003018-21-1	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
Data File : BF133811.D
Acq On : 16 Jun 2023 17:30
Operator : CG\JU
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Misc :
ALS Vial : 9 Sample Multiplier: 1

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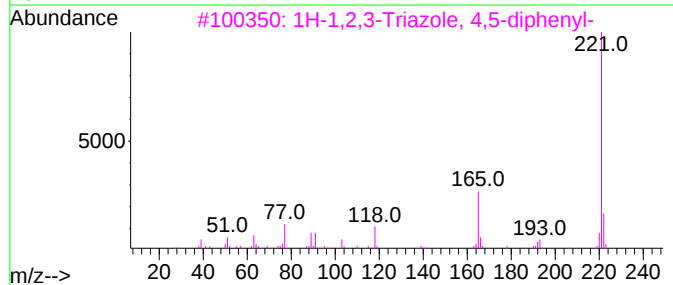
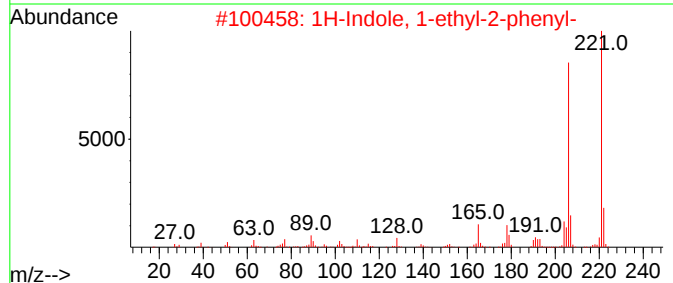
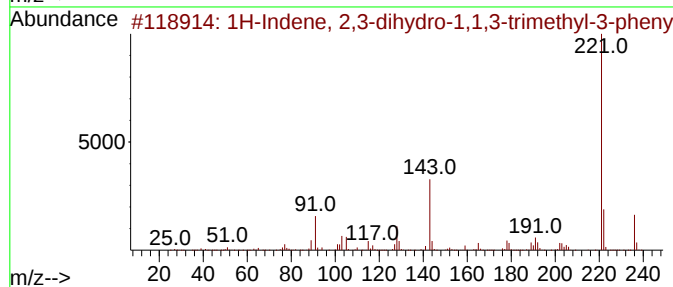
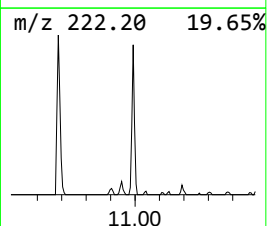
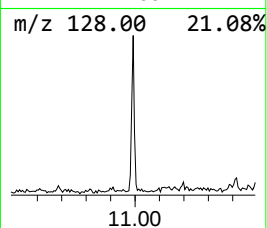
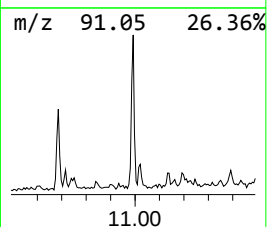
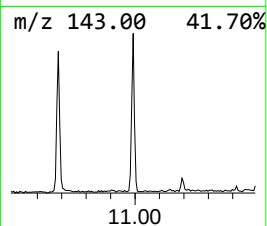
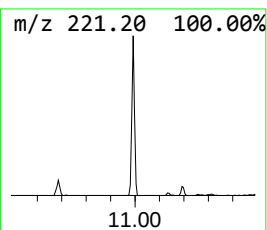
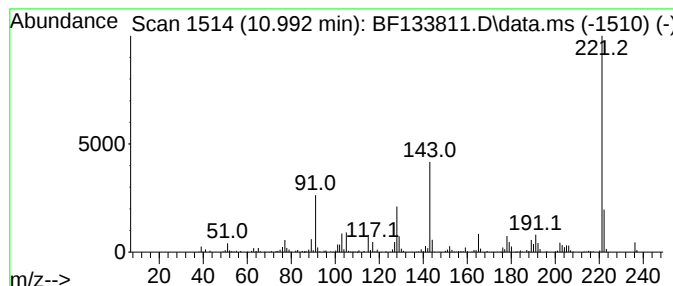
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1H-Indole, 1-ethyl-2-phenyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.992	7.68 ng	255003	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	72
2			1H-Indole, 1-ethyl-2-phenyl-	221	C16H15N	013228-39-2	49
3			1H-1,2,3-Triazole, 4,5-diphenyl-	221	C14H11N3	005533-73-3	47
4			Benzo[h]quinoline, 2,3,4-trimethyl-	221	C16H15N	063042-66-0	43
5			2-Pentene, 4-methyl-2,4-diphenyl-	236	C18H20	006258-73-7	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
Data File : BF133811.D
Acq On : 16 Jun 2023 17:30
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Misc :
ALS Vial : 9 Sample Multiplier: 1

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ClientSampleId :
COMPOSIT-SB-16

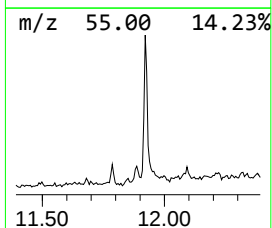
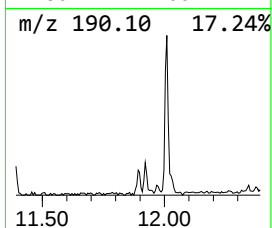
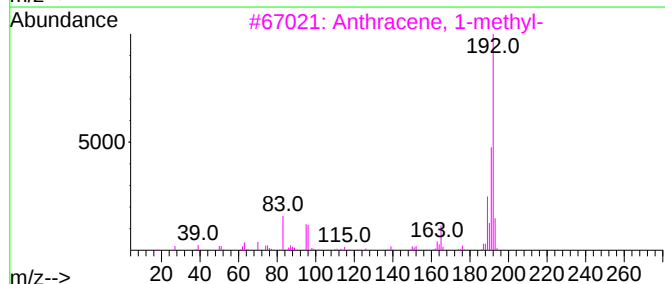
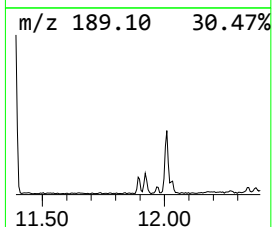
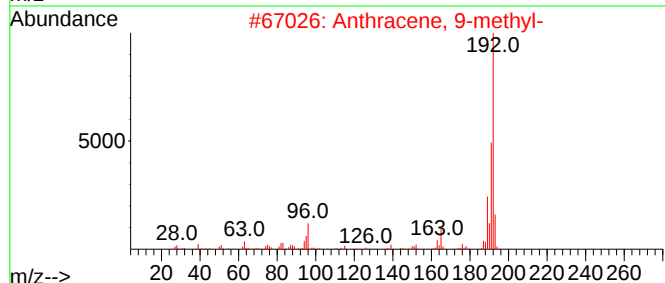
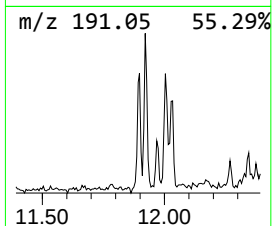
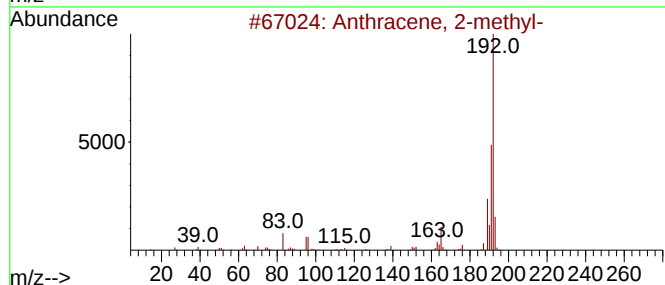
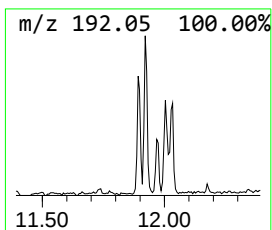
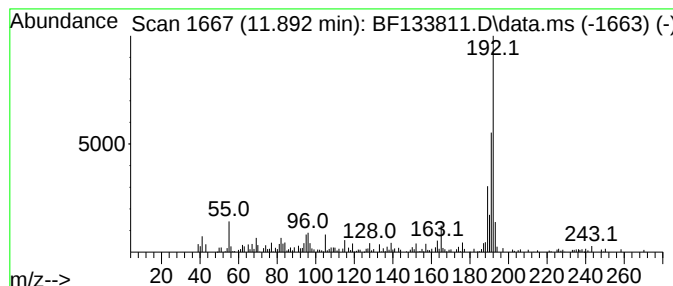
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Anthracene, 2-methyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	3.00 ng	99753	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
2			Anthracene, 9-methyl-	192	C15H12	000779-02-2	93
3			Anthracene, 1-methyl-	192	C15H12	000610-48-0	91
4			Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	90
5			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
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Misc :
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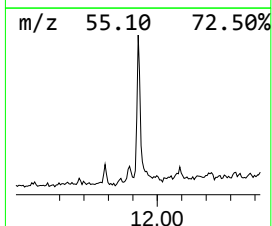
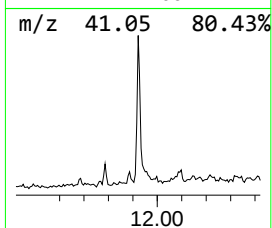
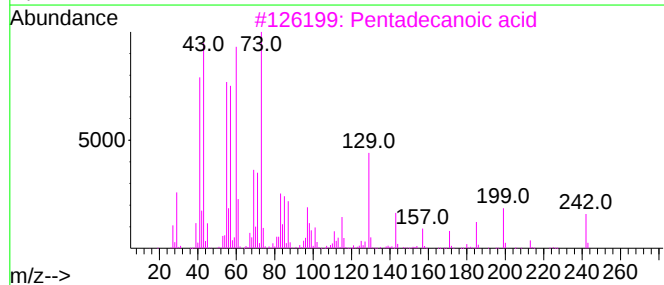
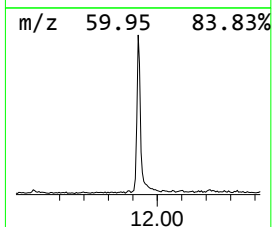
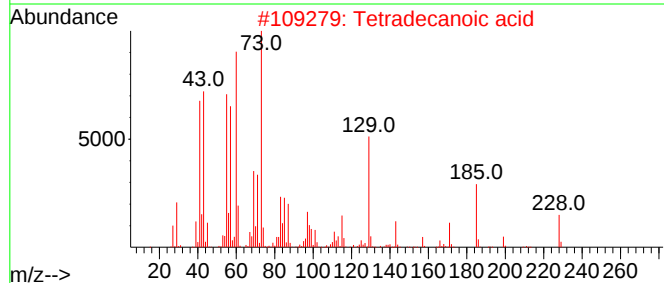
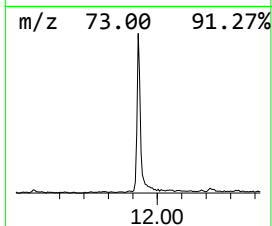
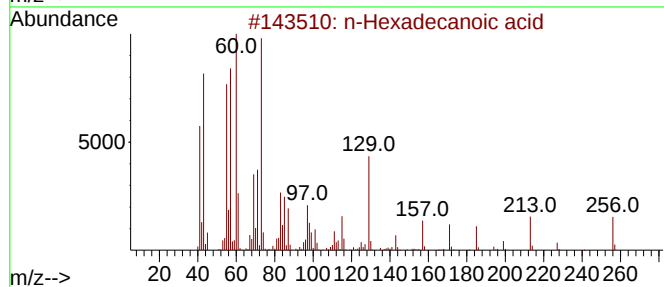
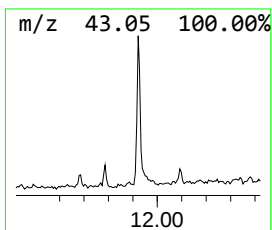
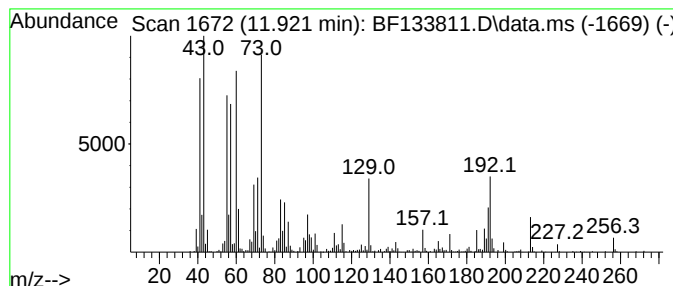
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	18.97 ng	630027	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4			Tridecanoic acid	214	C13H26O2	000638-53-9	60
5			n-Decanoic acid	172	C10H20O2	000334-48-5	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
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ALS Vial : 9 Sample Multiplier: 1

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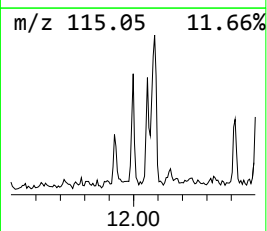
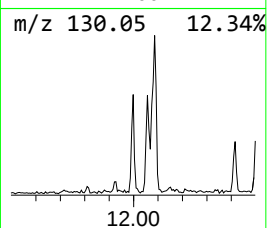
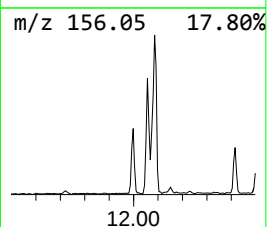
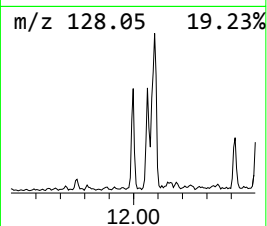
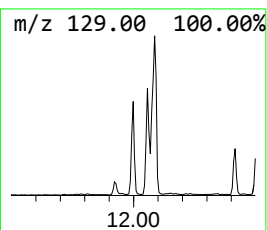
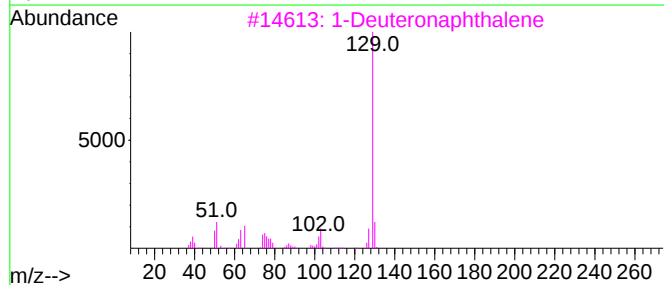
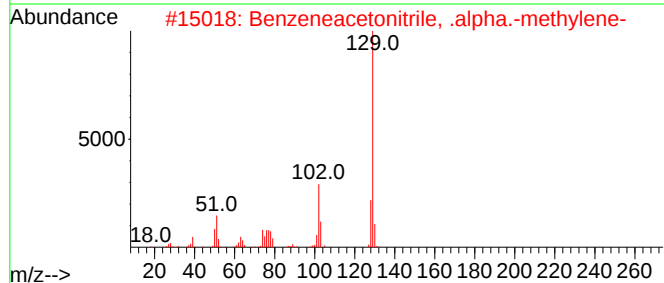
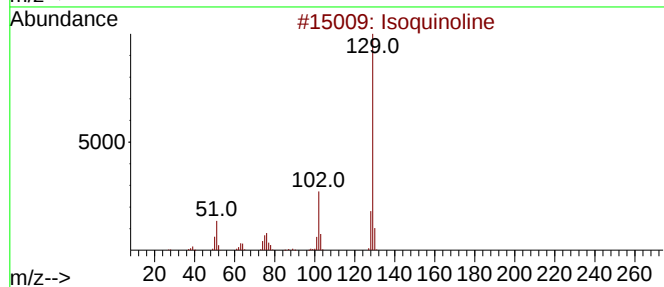
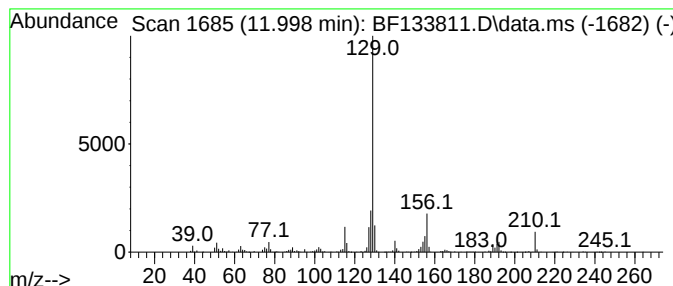
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Isoquinoline Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.998	10.35 ng	343848	Phenanthrene-d10	11.392

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isoquinoline	129	C9H7N	000119-65-3	52
2		Benzeneacetonitrile, .alpha.-met...	129	C9H7N	000495-10-3	50
3		1-Deuteronaphthalene	129	C10H7D	000875-62-7	47
4		Cyclohexanecarboxylic acid, hept...	226	C14H26O2	092319-47-6	38
5		2-Phenyl-2-(prop-2-en-1-yl)pent...	197	C14H15N	028049-67-4	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
Data File : BF133811.D
Acq On : 16 Jun 2023 17:30
Operator : CG\JU
Sample : 03222-19 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-16

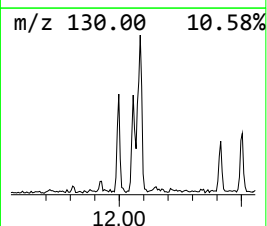
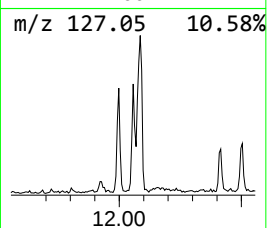
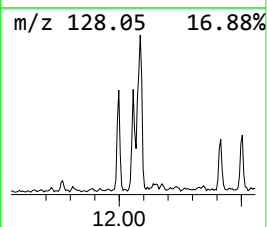
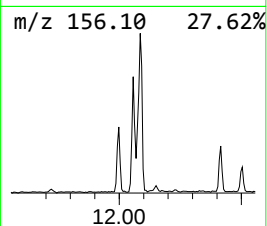
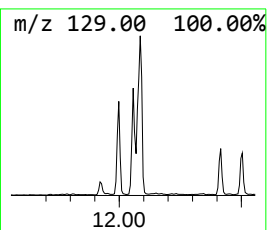
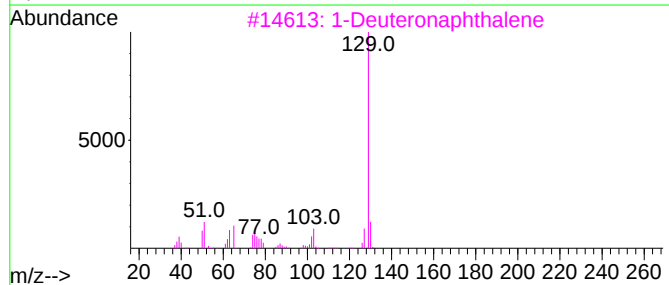
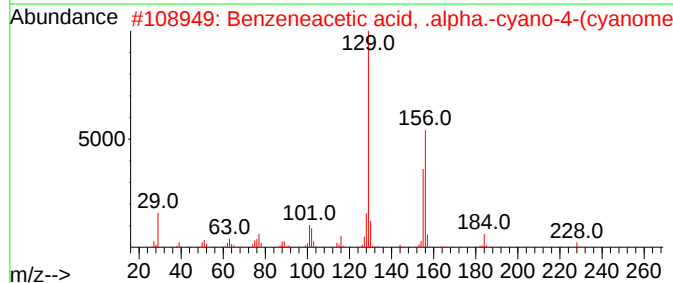
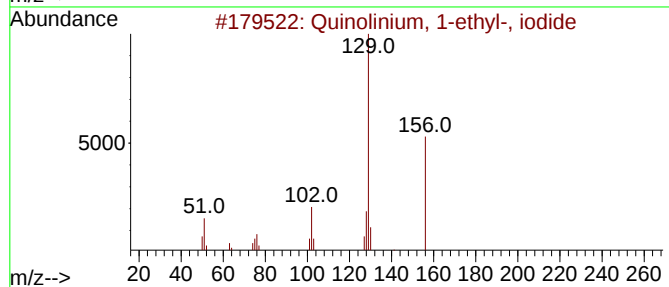
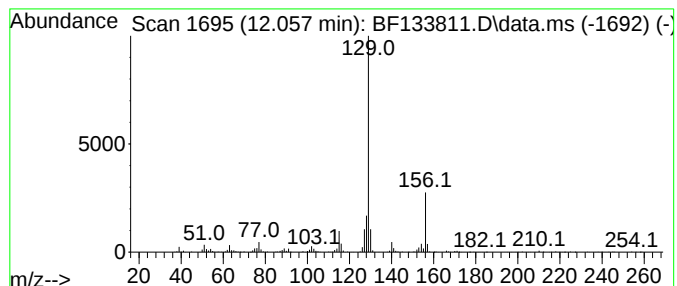
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Quinolinium, 1-ethyl-, iodide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.057	9.35 ng	310430	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Quinolinium, 1-ethyl-, iodide	285	C11H12IN	000634-35-5	64
2			Benzeneacetic acid, .alpha.-cyan...	228	C13H12N2O2	134882-04-5	50
3			1-Deuteronaphthalene	129	C10H7D	000875-62-7	47
4			Isoquinoline	129	C9H7N	000119-65-3	47
5			1,2-Benzenediacetonitrile	156	C10H8N2	000613-73-0	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
Data File : BF133811.D
Acq On : 16 Jun 2023 17:30
Operator : CG\JU
Sample : 03222-19 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-16

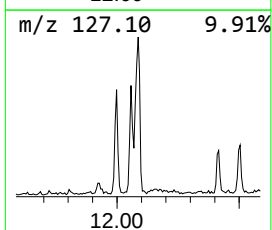
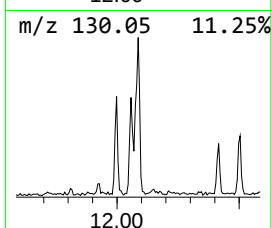
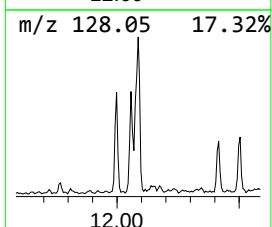
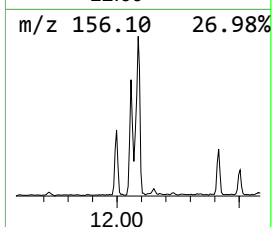
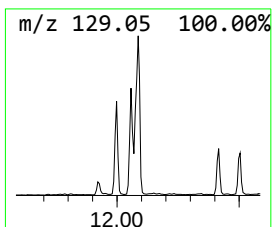
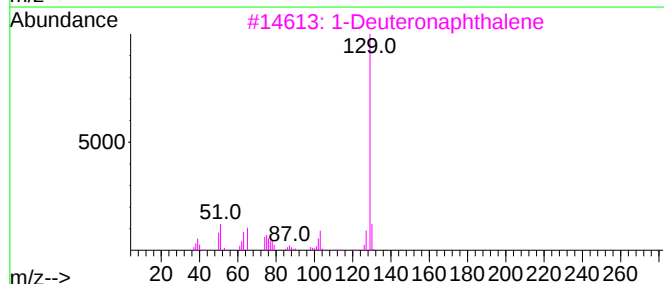
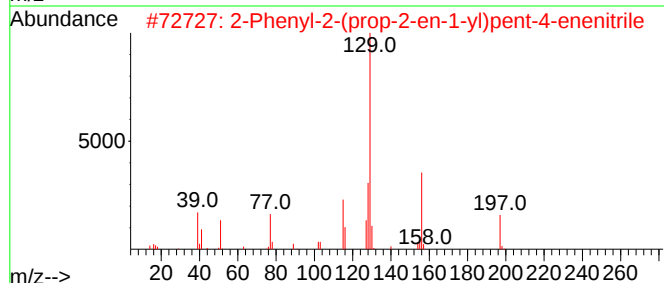
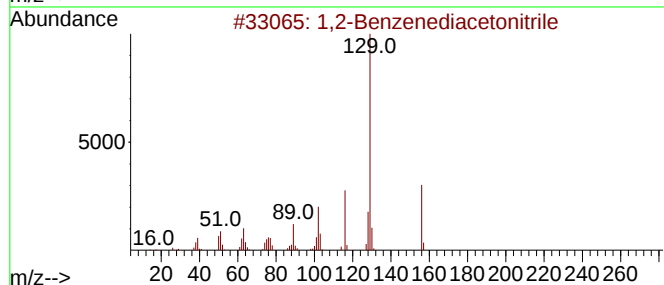
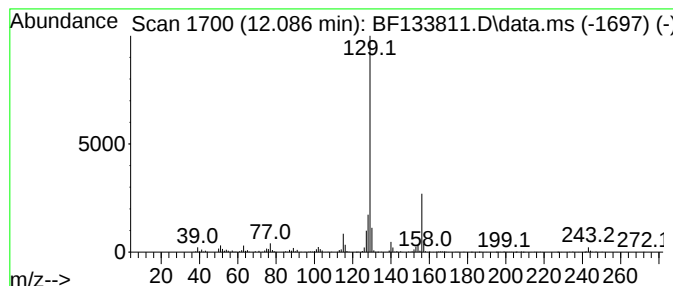
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1,2-Benzenediacetonitrile Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.086	18.08 ng	600528	Phenanthrene-d10	11.392

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,2-Benzenediacetonitrile	156	C10H8N2	000613-73-0	72
2		2-Phenyl-2-(prop-2-en-1-yl)pent-...	197	C14H15N	028049-67-4	56
3		1-Deuteronaphthalene	129	C10H7D	000875-62-7	50
4		Isoquinoline	129	C9H7N	000119-65-3	50
5		Naphthalene, 1,2-dihydro-2-methyl-	144	C11H12	021564-79-4	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
Data File : BF133811.D
Acq On : 16 Jun 2023 17:30
Operator : CG\JU
Sample : 03222-19 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
COMPOSIT-SB-16

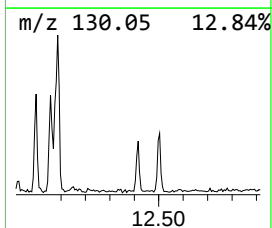
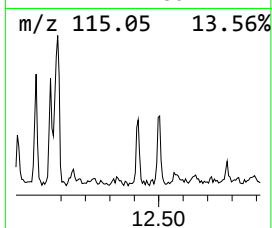
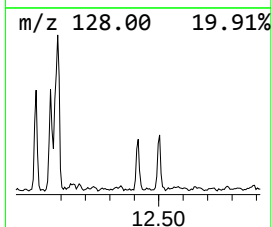
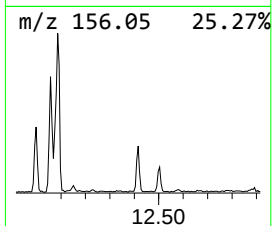
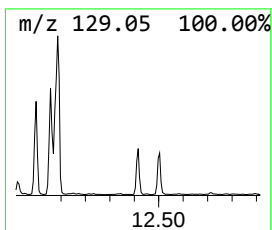
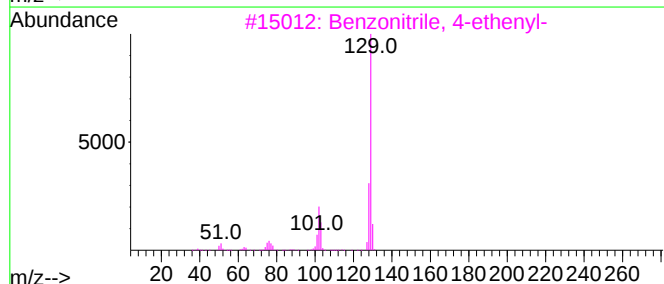
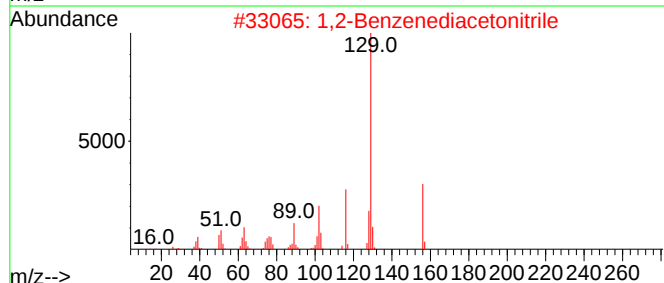
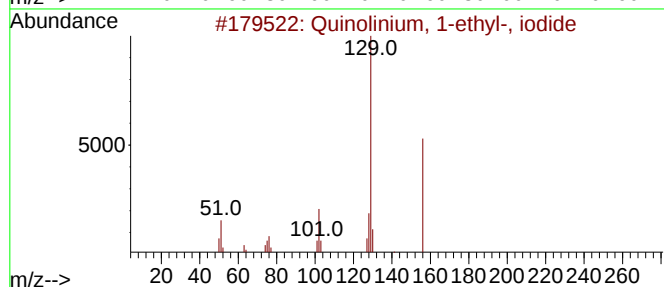
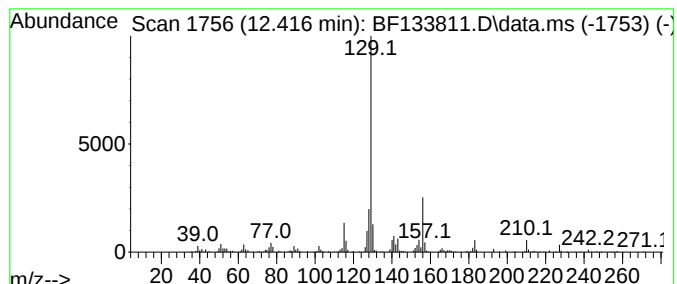
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Quinoline Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.416	4.38 ng	145609	Phenanthrene-d10	11.392

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Quinolinium, 1-ethyl-, iodide	285	C11H12IN	000634-35-5	72
2		1,2-Benzenediacetonitrile	156	C10H8N2	000613-73-0	64
3		Benzonitrile, 4-ethenyl-	129	C9H7N	003435-51-6	58
4		Quinoline	129	C9H7N	000091-22-5	50
5		Isoquinoline	129	C9H7N	000119-65-3	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
Data File : BF133811.D
Acq On : 16 Jun 2023 17:30
Operator : CG\JU
Sample : 03222-19 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

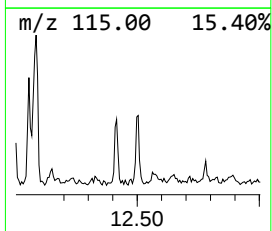
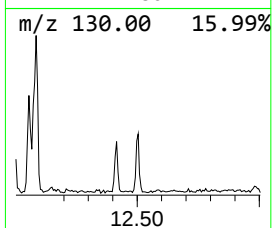
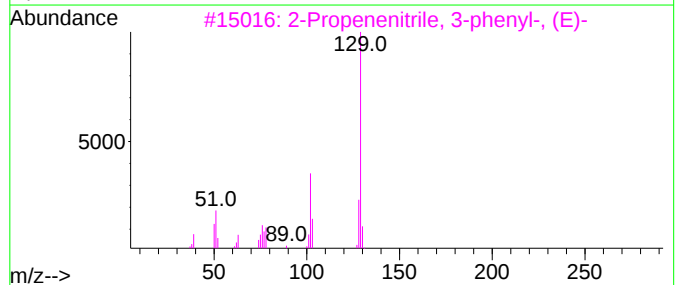
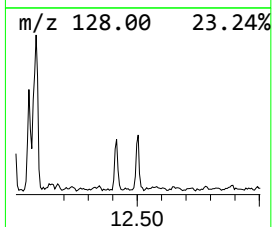
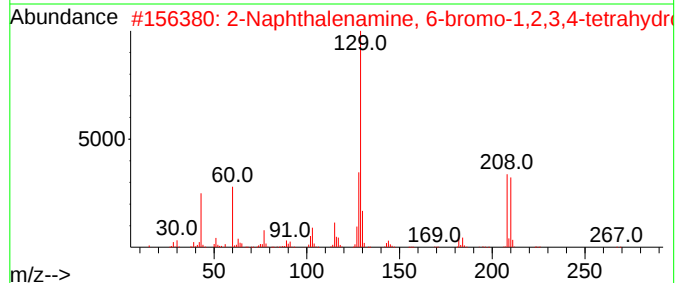
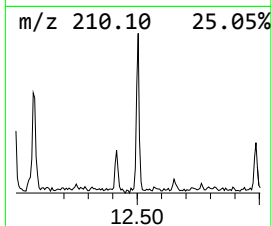
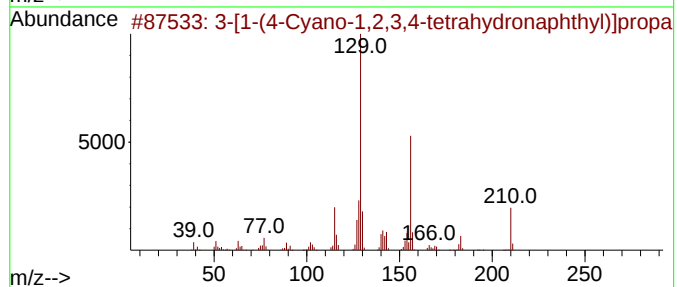
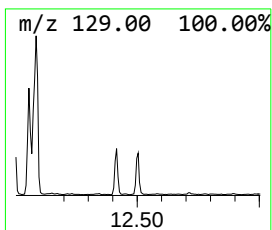
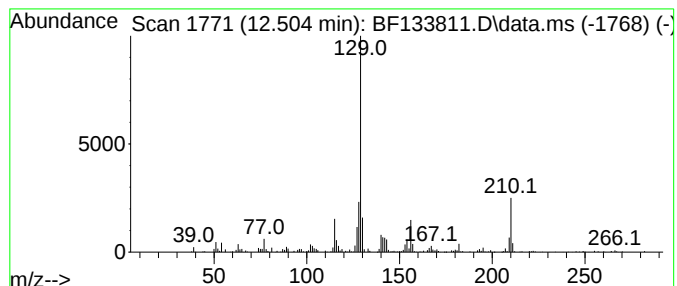
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ClientSampleId :
COMPOSIT-SB-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 3-[1-(4-Cyano-1,2,3,4-tetra... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD			R.T.
12.504	5.66 ng	187923	Phenanthrene-d10			11.392
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	3-[1-(4-Cyano-1,2,3,4-tetrahydro...		210	C14H14N2	057964-40-6	70
2	2-Naphthalenamine, 6-bromo-1,2,3...		267	C12H14BrNO	1000506-49-4	50
3	2-Propenenitrile, 3-phenyl-, (E)-		129	C9H7N	001885-38-7	50
4	Benzeneacetonitrile, .alpha.-met...		129	C9H7N	000495-10-3	50
5	Benzene, 1,3-hexadienyl-		158	C12H14	041635-77-2	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
Data File : BF133811.D
Acq On : 16 Jun 2023 17:30
Operator : CG\JU
Sample : 03222-19 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-16

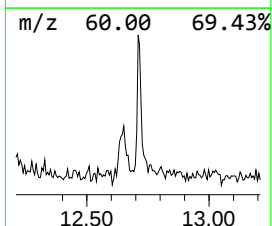
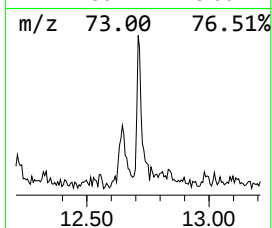
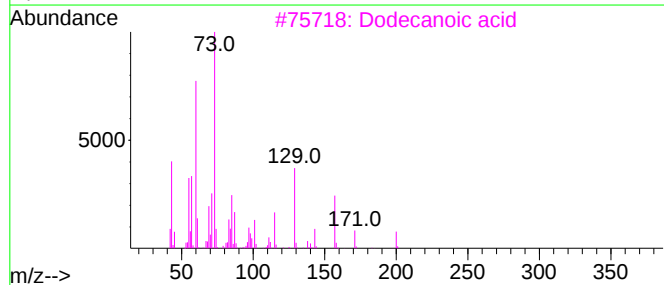
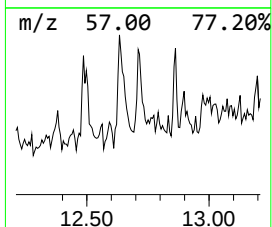
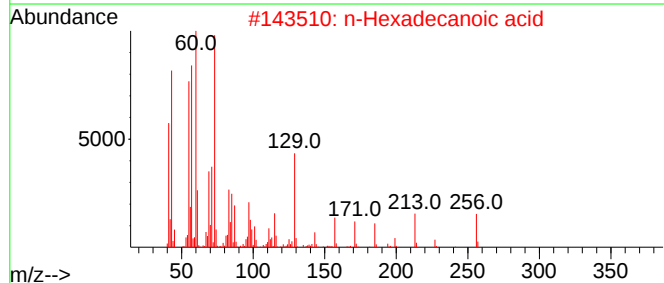
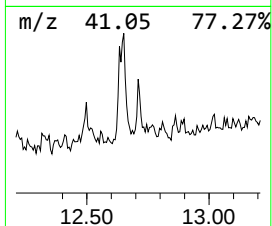
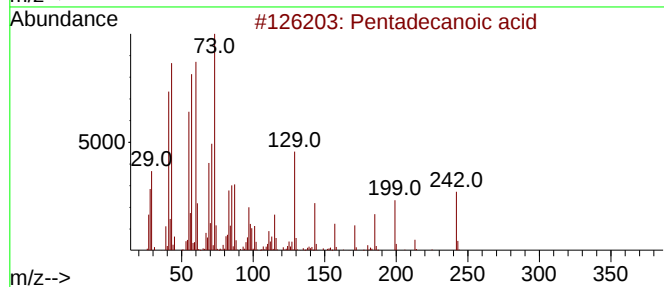
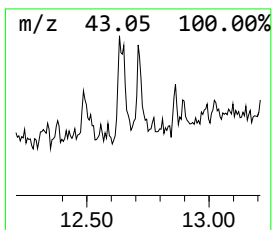
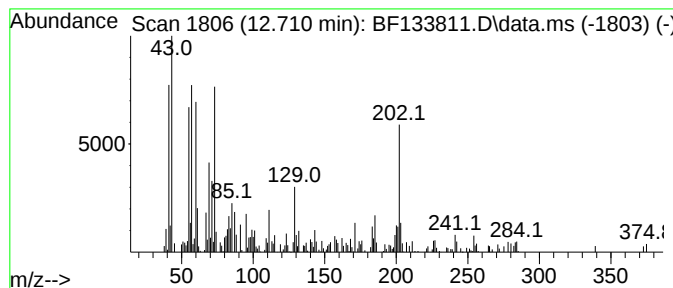
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 Pentadecanoic acid Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.710	3.08 ng	102280	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
3			Dodecanoic acid	200	C12H24O2	000143-07-7	55
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	49
5			Octadecanoic acid	284	C18H36O2	000057-11-4	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
COMPOSIT-SB-16

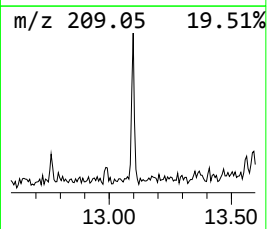
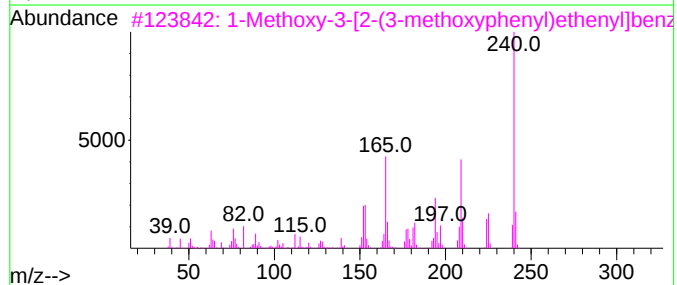
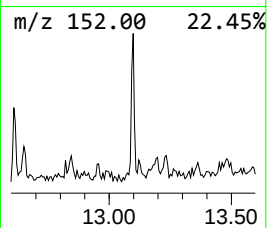
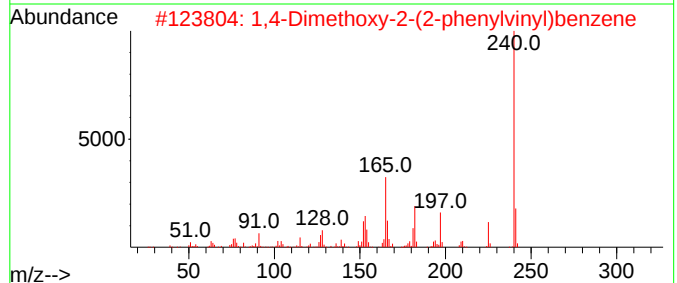
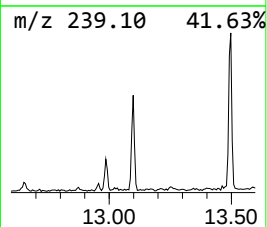
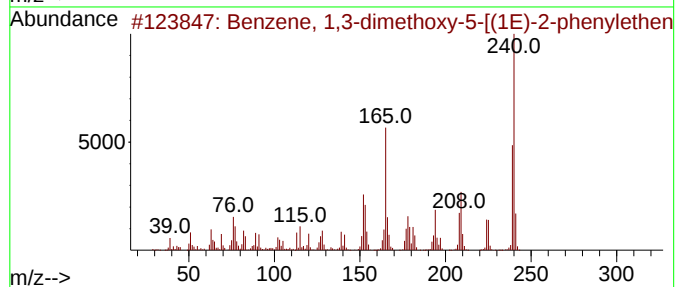
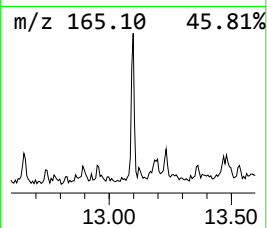
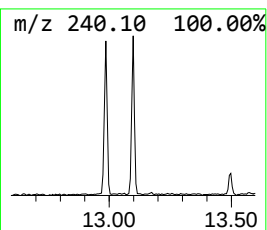
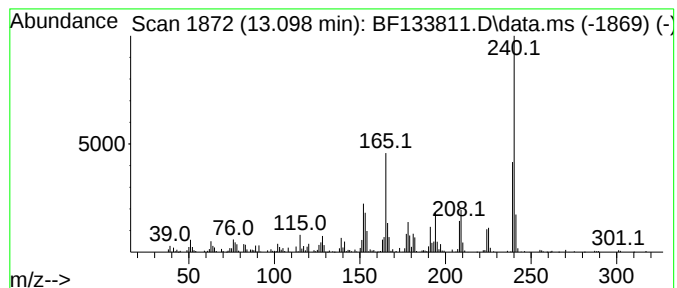
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Benzene, 1,3-dimethoxy-5-[(... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.098	3.86 ng	177341	Chrysene-d12	14.051

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1,3-dimethoxy-5-[(1E)-2...	240	C16H16O2	021956-56-9	98
2		1,4-Dimethoxy-2-(2-phenylvinyl)b...	240	C16H16O2	021889-09-8	90
3		1-Methoxy-3-[2-(3-methoxyphenyl)...]	240	C16H16O2	006325-63-9	89
4		Benzene, 1,3-dimethoxy-4-[(1E)-2...	240	C16H16O2	1000368-46-0	50
5		[1,1'-Biphenyl]-4,4'-diamine, 3,...	240	C16H20N2	054827-17-7	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
Data File : BF133811.D
Acq On : 16 Jun 2023 17:30
Operator : CG\JU
Sample : 03222-19 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-16

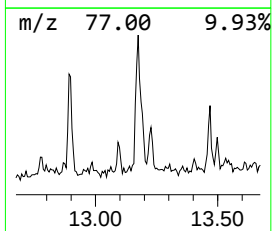
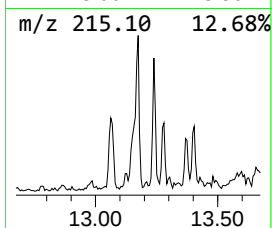
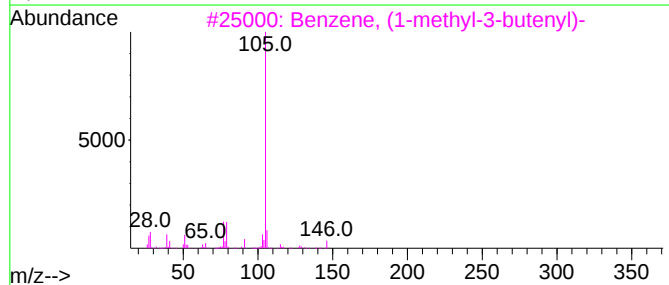
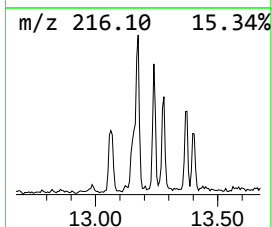
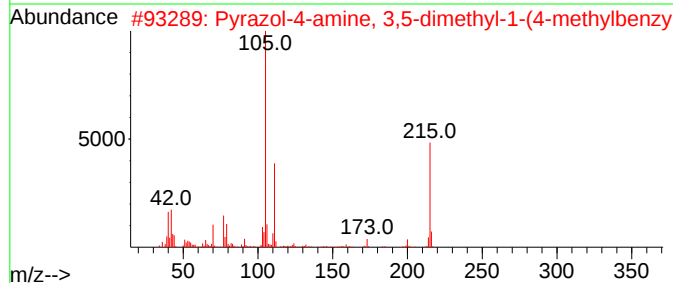
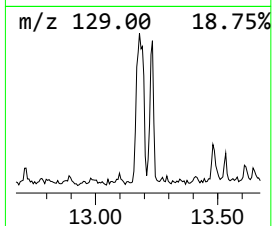
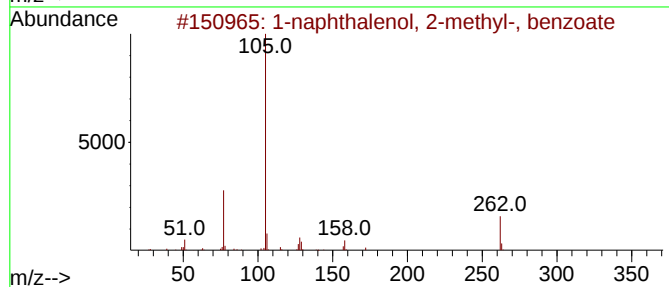
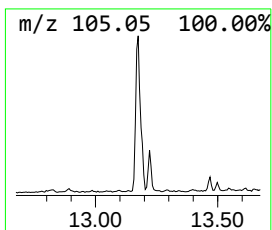
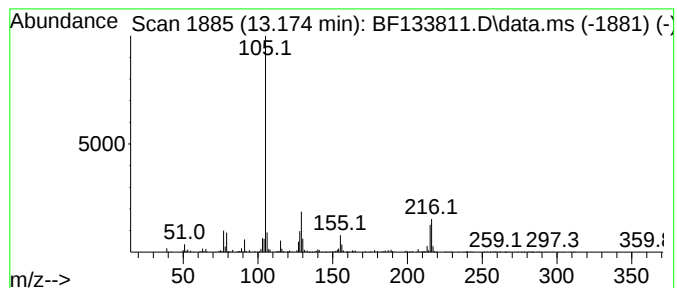
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 unknown13.174 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.174	10.00 ng	458907	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-naphthalenol, 2-methyl-, benzoate	262	C18H14O2	1010396-82-6	43
2			Pyrazol-4-amine, 3,5-dimethyl-1-(4-methylbenzyl)-	215	C13H17N3	1000272-85-6	22
3			Benzene, (1-methyl-3-butenyl)-	146	C11H14	010340-49-5	22
4			Hydratropic acid, 3-methylbut-2-en-1-yl 4-methylbenzoate	218	C14H18O2	1000406-95-5	18
5			1-Phenylethanethiol, S-(2-methylbut-3-en-1-yl)	208	C12H16OS	1227931-65-8	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
Data File : BF133811.D
Acq On : 16 Jun 2023 17:30
Operator : CG\JU
Sample : 03222-19 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-16

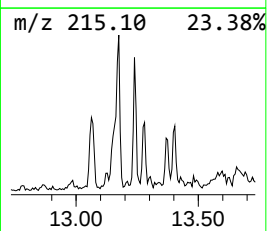
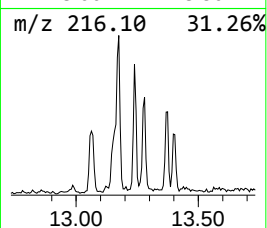
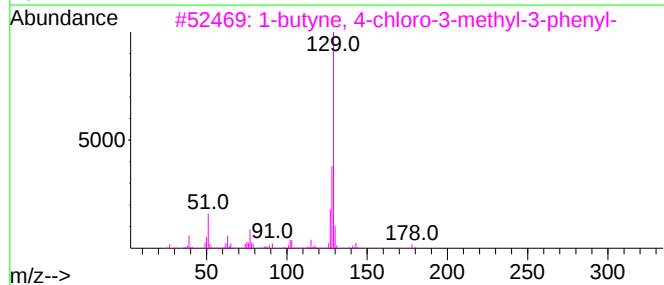
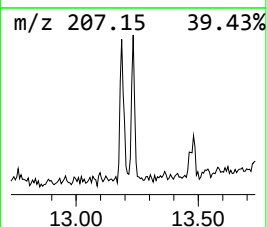
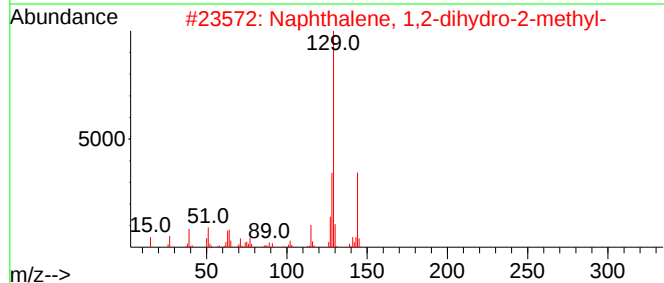
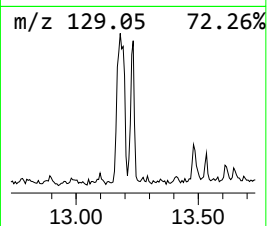
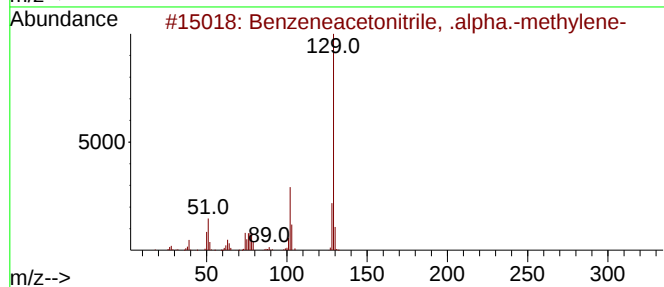
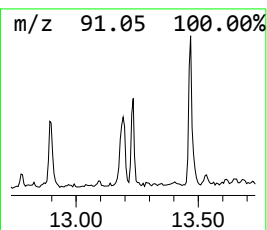
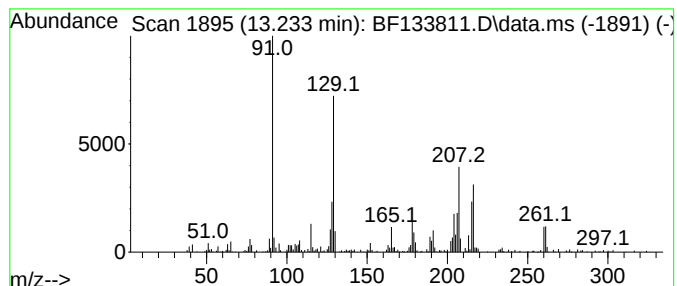
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown13.233 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.233	4.13 ng	189760	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneacetonitrile, .alpha.-met...	129	C9H7N	000495-10-3	14
2			Naphthalene, 1,2-dihydro-2-methyl-	144	C11H12	021564-79-4	14
3			1-butyne, 4-chloro-3-methyl-3-ph...	178	C11H11Cl	1000161-45-9	14
4			(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20O5	131758-71-9	12
5			6-Methoxy-6-oxohexan-2-yl (E)-2,...	422	C22H30O8	1000495-80-7	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
Data File : BF133811.D
Acq On : 16 Jun 2023 17:30
Operator : CG\JU
Sample : 03222-19 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

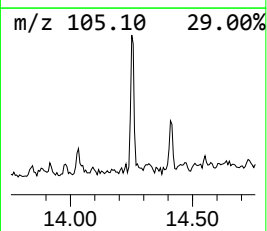
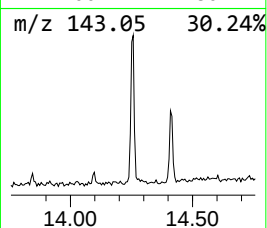
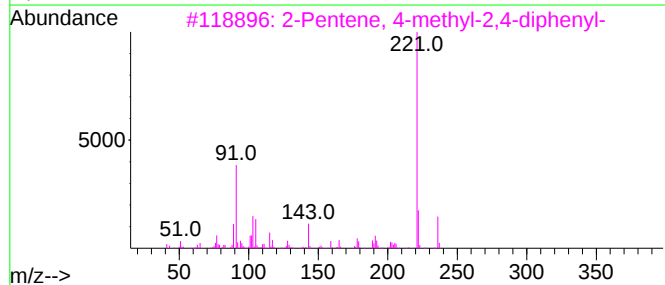
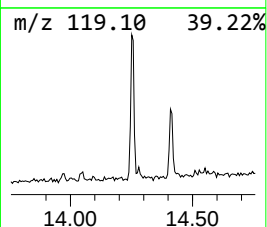
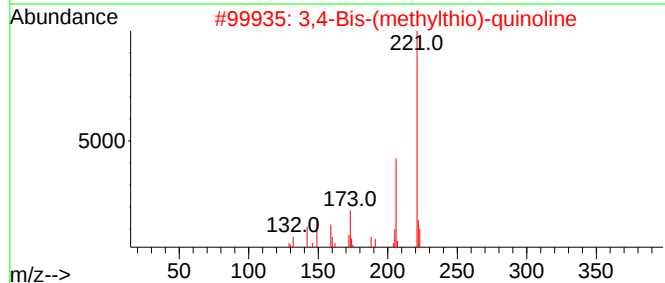
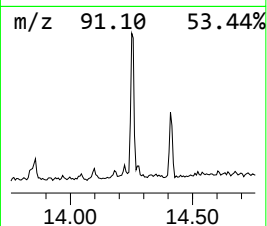
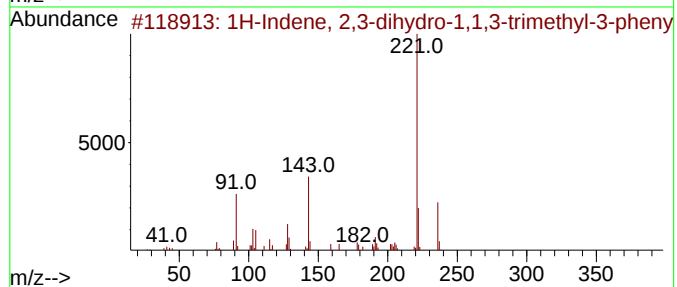
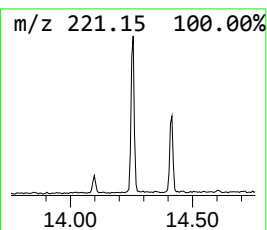
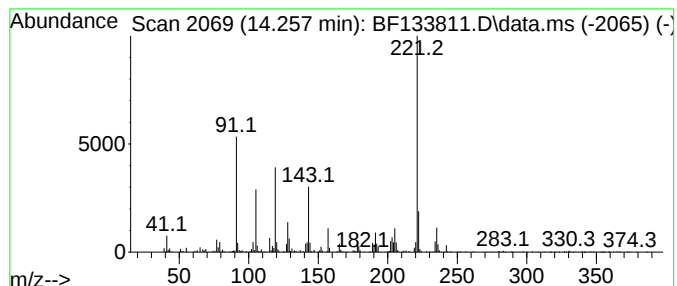
Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 1H-Indene, 2,3-dihydro-1,1,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD			R.T.
14.257	8.25 ng	378783	Chrysene-d12			14.051
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	52
2		3,4-Bis-(methylthio)-quinoline	221	C11H11NS2	074579-34-3	50
3		2-Pentene, 4-methyl-2,4-diphenyl-	236	C18H20	006258-73-7	47
4		Indole, 5-(4-methylphenyl)-N-met...	221	C16H15N	1000380-54-7	46
5		2-Mercapto-4,6-dimethylnicotinon...	236	C11H16N2SSi	1000332-43-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
Data File : BF133811.D
Acq On : 16 Jun 2023 17:30
Operator : CG\JU
Sample : 03222-19 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-16

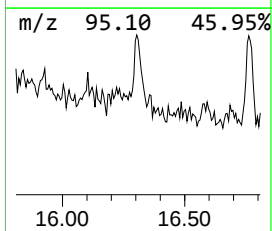
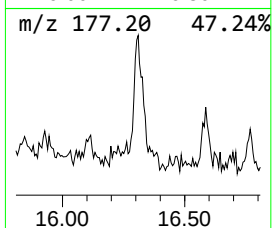
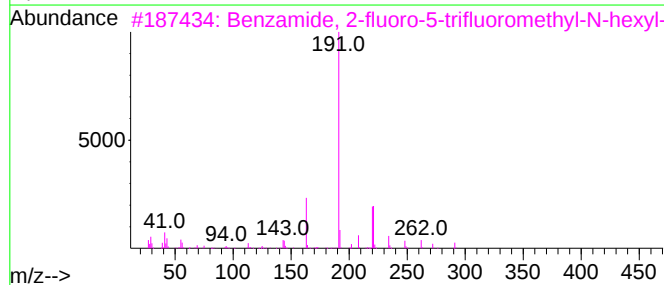
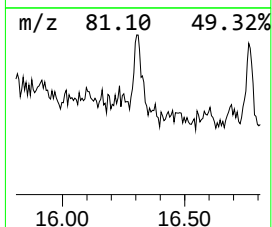
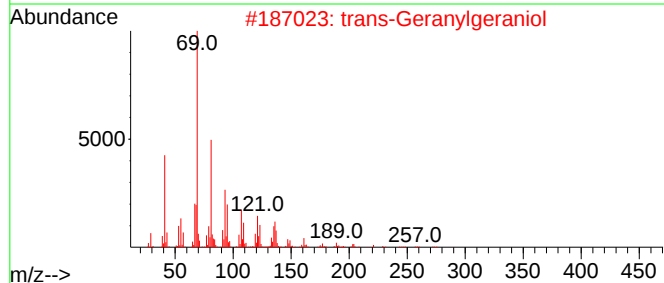
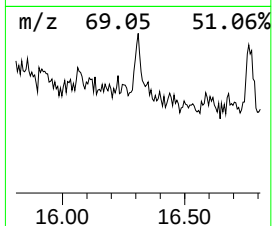
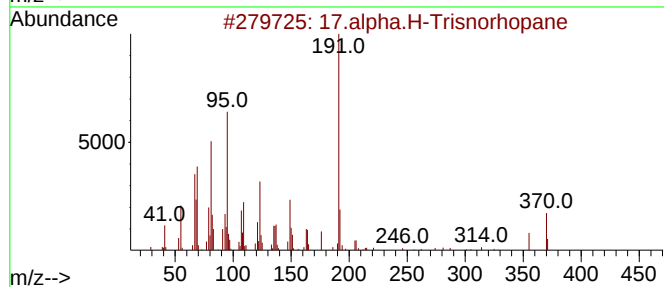
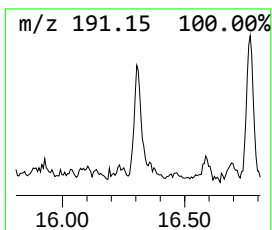
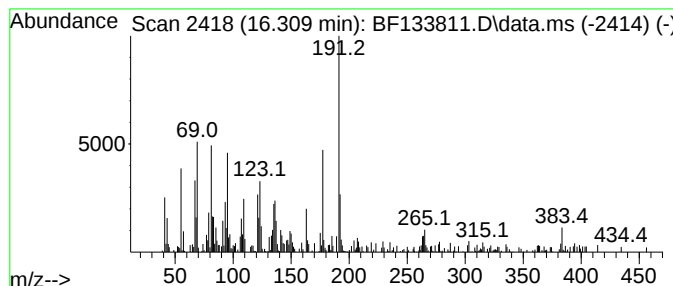
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 unknown16.309 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.309	23.59 ng	328747	Perylene-d12	15.562

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		17.alpha.H-Trisnorhopane	370	C27H46	053584-59-1	49
2		trans-Geranylgeraniol	290	C20H34O	024034-73-9	35
3		Benzamide, 2-fluoro-5-trifluorom...	291	C14H17F4NO	1000420-17-2	30
4		Furan-2-carboxylic acid, 5-bromo...	393	C18H20BrNO4	1000311-01-7	30
5		1-(3-Nitro-phenyl)-pyrrolidine	192	C10H12N2O2	1000300-34-7	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
 Data File : BF133811.D
 Acq On : 16 Jun 2023 17:30
 Operator : CG\JU
 Sample : 03222-19 2X
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSIT-SB-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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
Butane, 2-metho...	2.116	11.7	ng	286288	1	6.863	488600	20.0
1,3,5-Cyclohept...	3.957	4.9	ng	120491	1	6.863	488600	20.0
Ethylbenzene	5.357	12.1	ng	295115	1	6.863	488600	20.0
Styrene	5.710	31.1	ng	758758	1	6.863	488600	20.0
Benzophenone	10.610	5.3	ng	196663	3	9.898	745818	20.0
unknown10.933	10.933	3.1	ng	102419	4	11.392	664262	20.0
1H-Indole, 1-et...	10.992	7.7	ng	255003	4	11.392	664262	20.0
Anthracene, 2-m...	11.892	3.0	ng	99753	4	11.392	664262	20.0
n-Hexadecanoic ...	11.922	19.0	ng	630027	4	11.392	664262	20.0
Isoquinoline	11.998	10.4	ng	343848	4	11.392	664262	20.0
Quinolinium, 1-...	12.057	9.3	ng	310430	4	11.392	664262	20.0
1,2-Benzenediac...	12.086	18.1	ng	600528	4	11.392	664262	20.0
Quinoline	12.416	4.4	ng	145609	4	11.392	664262	20.0
3-[1-(4-Cyano-1...	12.504	5.7	ng	187923	4	11.392	664262	20.0
Pentadecanoic acid	12.710	3.1	ng	102280	4	11.392	664262	20.0
Benzene, 1,3-di...	13.098	3.9	ng	177341	5	14.051	918155	20.0
unknown13.174	13.174	10.0	ng	458907	5	14.051	918155	20.0
unknown13.233	13.233	4.1	ng	189760	5	14.051	918155	20.0
1H-Indene, 2,3-...	14.257	8.3	ng	378783	5	14.051	918155	20.0
unknown16.309	16.309	23.6	ng	328747	6	15.562	278727	20.0