

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101923\
 Data File : BF135893.D
 Acq On : 19 Oct 2023 18:46
 Operator : CG\JU
 Sample : 04907-01 2X
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OR-03-101623

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-BF101323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135893.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.340	379	383	389	rBV6	6409	11375	1.80%	0.145%
2	4.916	477	481	483	rBV2	23517	26781	4.24%	0.342%
3	4.940	483	485	499	rVB	191401	247798	39.28%	3.163%
4	5.122	513	516	521	rBV3	8684	9506	1.51%	0.121%
5	5.375	556	559	574	rBV	412753	630908	100.00%	8.054%
6	5.487	576	578	583	rVB3	11974	16125	2.56%	0.206%
7	5.734	615	620	621	rBV4	8929	12109	1.92%	0.155%
8	5.875	641	644	649	rVB3	9425	9559	1.52%	0.122%
9	5.975	658	661	663	rBV2	7946	9103	1.44%	0.116%
10	6.157	687	692	696	rBV4	6597	7890	1.25%	0.101%
11	6.251	705	708	715	rBV	28062	29712	4.71%	0.379%
12	6.392	729	732	744	rBV	438966	591185	93.70%	7.547%
13	6.734	787	790	797	rBV	446719	376100	59.61%	4.801%
14	6.986	830	833	839	rBV4	12311	15575	2.47%	0.199%
15	7.245	872	877	879	rBV6	9450	13465	2.13%	0.172%
16	7.304	884	887	901	rBV	434769	484492	76.79%	6.185%
17	7.639	942	944	948	rVB2	8943	8324	1.32%	0.106%
18	7.992	1001	1004	1005	rBV2	7912	7822	1.24%	0.100%
19	8.016	1005	1008	1015	rVV	495269	447527	70.93%	5.713%
20	8.069	1015	1017	1021	rVB	10461	9861	1.56%	0.126%
21	8.210	1038	1041	1044	rVB3	9040	7753	1.23%	0.099%
22	8.433	1074	1079	1080	rBV	12182	12827	2.03%	0.164%
23	8.751	1127	1133	1135	rBV5	6625	10038	1.59%	0.128%
24	9.033	1178	1181	1184	rBV	14486	11893	1.89%	0.152%
25	9.092	1187	1191	1198	rVV	634069	559089	88.62%	7.137%
26	9.169	1199	1204	1208	rVB3	13661	15420	2.44%	0.197%
27	9.210	1208	1211	1214	rBV2	13264	12036	1.91%	0.154%
28	9.463	1252	1254	1256	rBV	18516	16514	2.62%	0.211%
29	9.486	1256	1258	1261	rVB	19622	17192	2.72%	0.219%
30	9.633	1280	1283	1287	rVB4	14650	20598	3.26%	0.263%
31	9.669	1287	1289	1292	rVB2	17470	15576	2.47%	0.199%
32	9.698	1292	1294	1298	rBV3	12851	13393	2.12%	0.171%
33	9.739	1298	1301	1303	rBV3	9117	10663	1.69%	0.136%
34	9.769	1303	1306	1310	rVV	537761	469281	74.38%	5.991%
35	9.804	1310	1312	1315	rVB3	14756	14023	2.22%	0.179%
36	9.927	1329	1333	1336	rBV6	5942	8155	1.29%	0.104%

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Integrator: RTE

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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

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37	10.022	1346	1349	1352	rVB5	9244	9846	1.56%	0.126%
38	10.098	1357	1362	1364	rBV6	11535	14978	2.37%	0.191%
39	10.127	1364	1367	1372	rVB7	8172	11559	1.83%	0.148%
40	10.169	1372	1374	1378	rBV3	9622	9961	1.58%	0.127%
41	10.327	1398	1401	1404	rBV3	9205	10665	1.69%	0.136%
42	10.421	1413	1417	1422	rVB	14001	18175	2.88%	0.232%
43	10.569	1439	1442	1451	rBV	324152	330391	52.37%	4.218%
44	10.686	1458	1462	1465	rBV	28736	32648	5.17%	0.417%
45	10.886	1490	1496	1497	rBV6	7182	10215	1.62%	0.130%
46	11.127	1534	1537	1539	rBV3	8792	7926	1.26%	0.101%
47	11.157	1539	1542	1549	rVB2	16029	21717	3.44%	0.277%
48	11.269	1557	1561	1564	rBV	479289	416572	66.03%	5.318%
49	11.292	1564	1565	1571	rVB	97128	75850	12.02%	0.968%
50	11.351	1572	1575	1580	rBV	25386	24804	3.93%	0.317%
51	11.510	1599	1602	1603	rBV3	7299	7761	1.23%	0.099%
52	11.774	1645	1647	1649	rBV	19324	16503	2.62%	0.211%
53	11.804	1649	1652	1659	rVB3	83533	100408	15.91%	1.282%
54	11.886	1664	1666	1669	rVV	39571	39622	6.28%	0.506%
55	11.916	1669	1671	1677	rVB	16125	18899	3.00%	0.241%
56	11.968	1677	1680	1682	rBV4	8236	9580	1.52%	0.122%
57	12.016	1684	1688	1689	rBV4	6329	7146	1.13%	0.091%
58	12.074	1695	1698	1702	rBV2	14307	17533	2.78%	0.224%
59	12.127	1705	1707	1712	rVB5	8063	9445	1.50%	0.121%
60	12.257	1726	1729	1731	rBV3	10456	10607	1.68%	0.135%
61	12.327	1738	1741	1744	rBV	29518	29245	4.64%	0.373%
62	12.357	1744	1746	1749	rVV4	11940	15739	2.49%	0.201%
63	12.433	1754	1759	1761	rBV4	13797	26984	4.28%	0.344%
64	12.492	1766	1769	1774	rBV	217709	210718	33.40%	2.690%
65	12.598	1784	1787	1792	rBV5	21931	32628	5.17%	0.417%
66	12.645	1793	1795	1798	rVV2	18617	19602	3.11%	0.250%
67	12.721	1802	1808	1814	rBV	213570	272983	43.27%	3.485%
68	12.780	1815	1818	1821	rVB	23956	27678	4.39%	0.353%
69	12.863	1828	1832	1841	rVB	689023	601628	95.36%	7.680%
70	12.939	1843	1845	1846	rBV2	17208	11704	1.86%	0.149%
71	13.033	1858	1861	1862	rBV2	15309	14318	2.27%	0.183%
72	13.121	1874	1876	1879	rBV3	17586	16267	2.58%	0.208%
73	13.162	1880	1883	1887	rVV2	29363	30296	4.80%	0.387%
74	13.257	1896	1899	1901	rBV	25588	25305	4.01%	0.323%
75	13.433	1926	1929	1932	rBV4	20221	31485	4.99%	0.402%
76	13.933	2010	2014	2017	rBV2	329506	370227	58.68%	4.726%

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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

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Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	13.962	2017	2019	2025	rVB	66756	66058	10.47%	0.843%
78	15.415	2262	2266	2270	rVB	196541	233860	37.07%	2.985%
79	16.062	2372	2376	2382	rVB3	102659	181781	28.81%	2.321%
80	16.492	2446	2449	2458	rVB	115643	202437	32.09%	2.584%

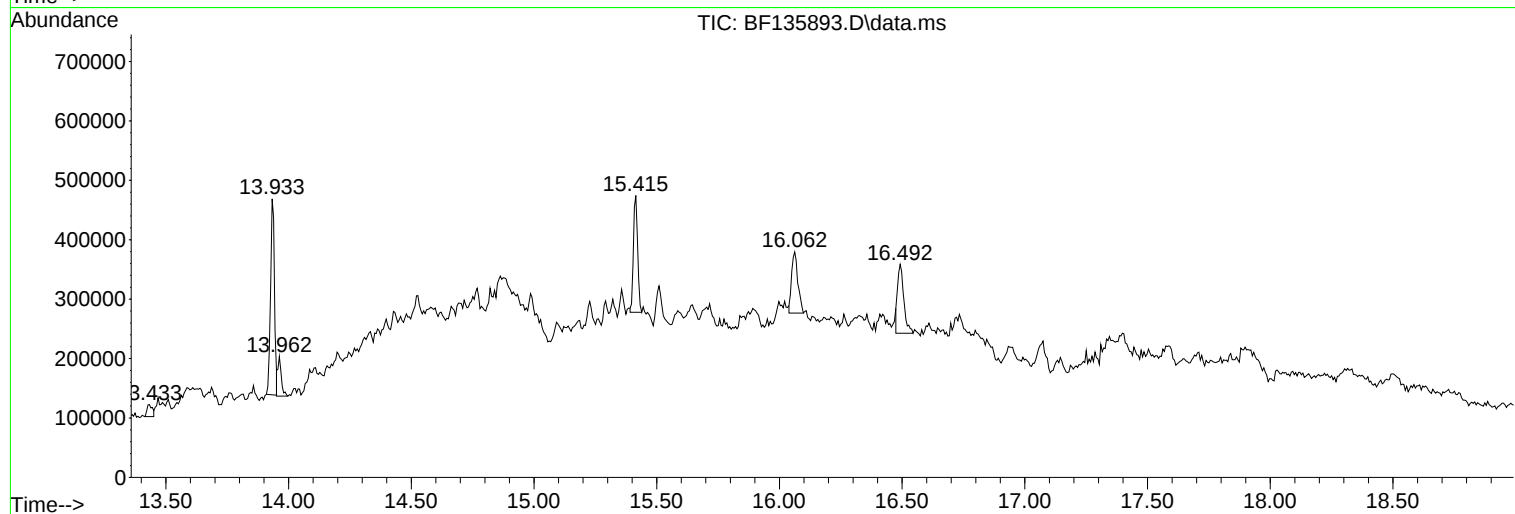
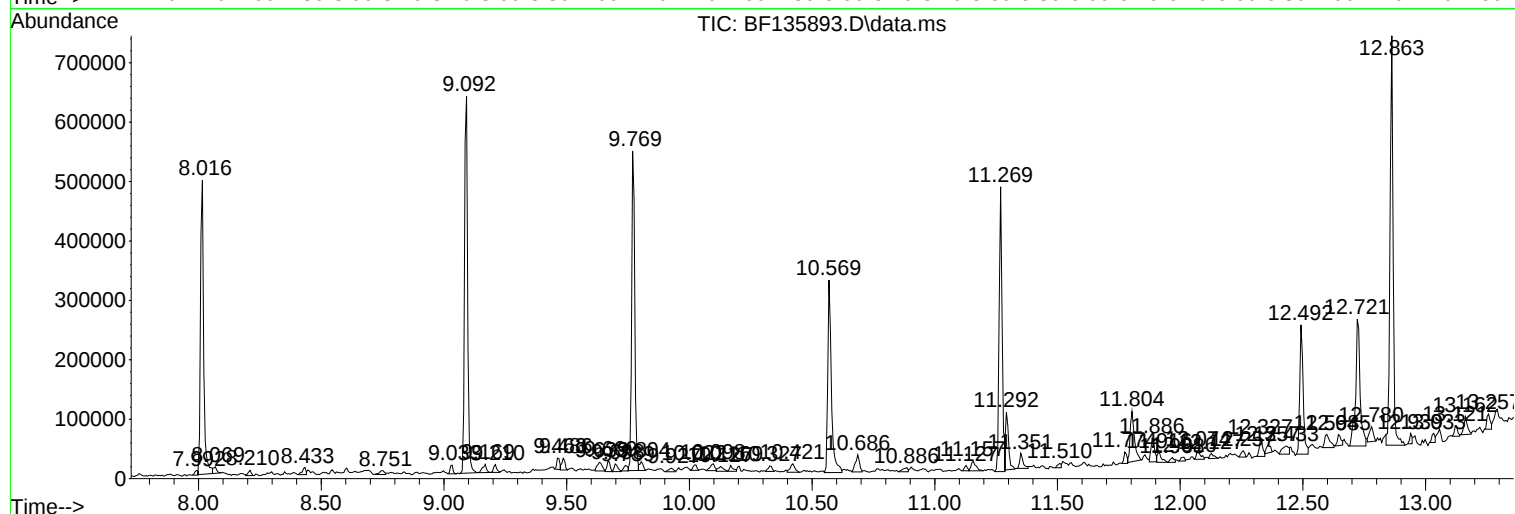
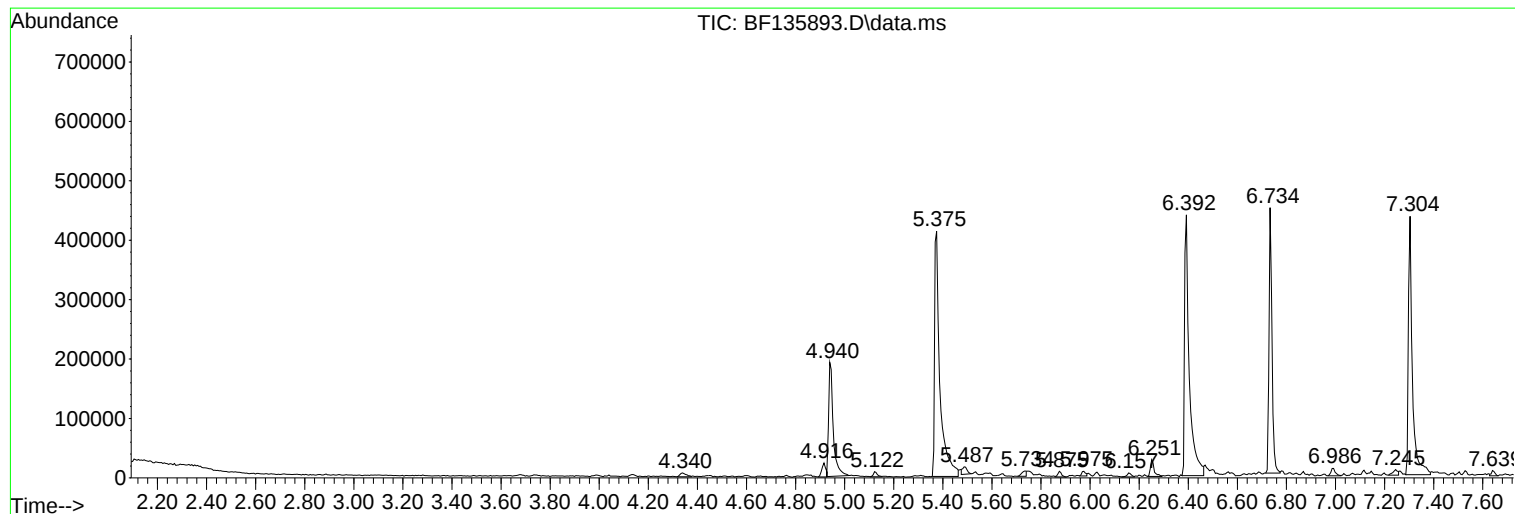
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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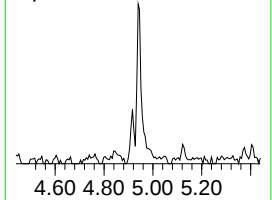
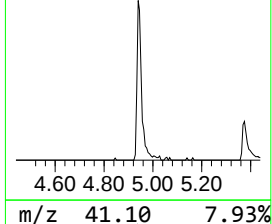
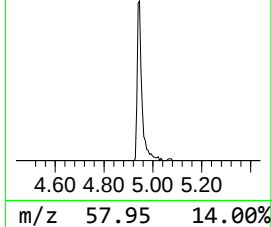
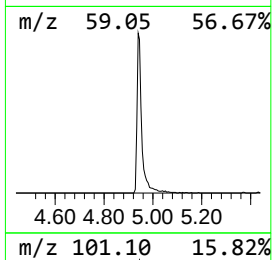
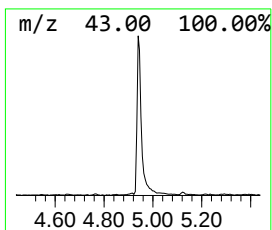
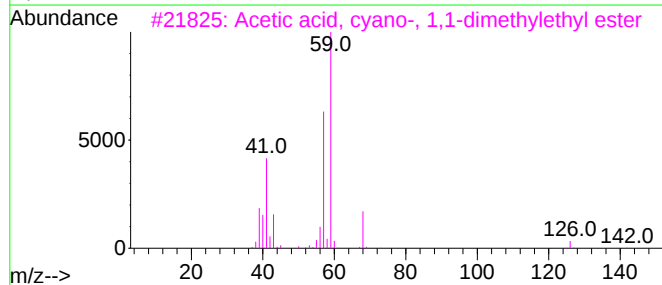
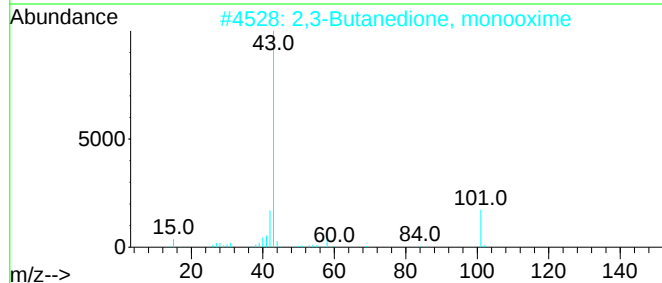
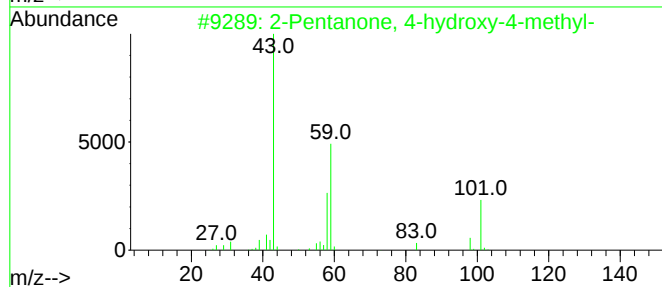
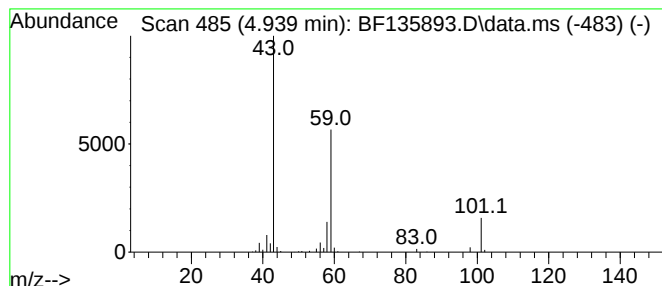
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.939	13.18 ng	247798	1,4-Dichlorobenzene-d4	6.734

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	9		



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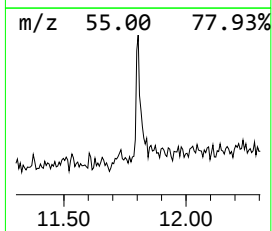
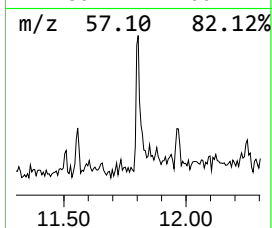
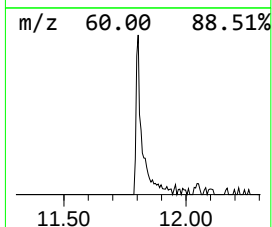
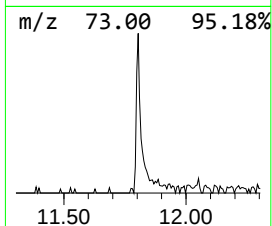
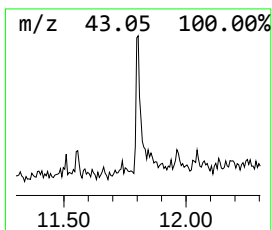
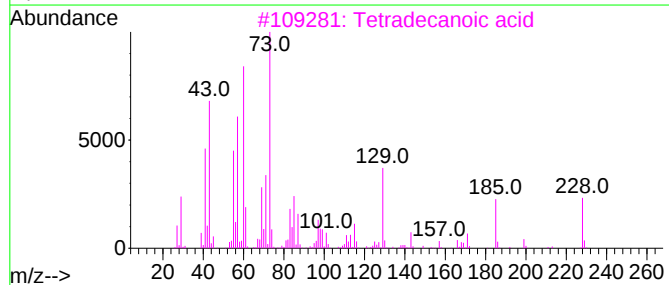
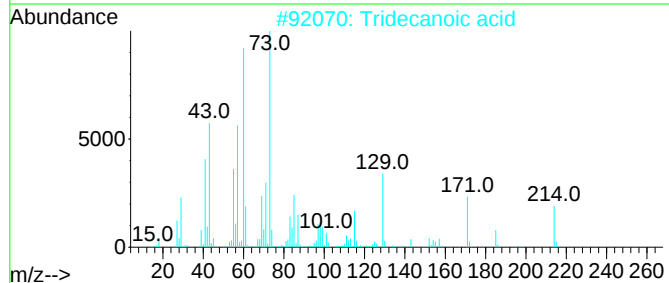
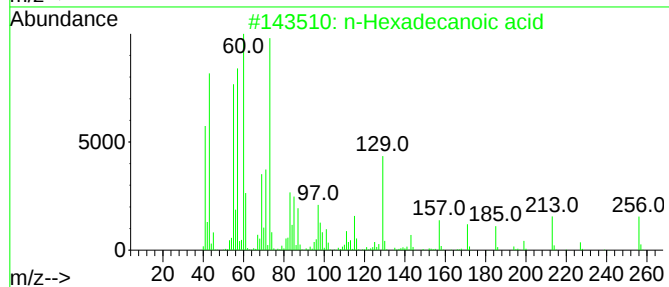
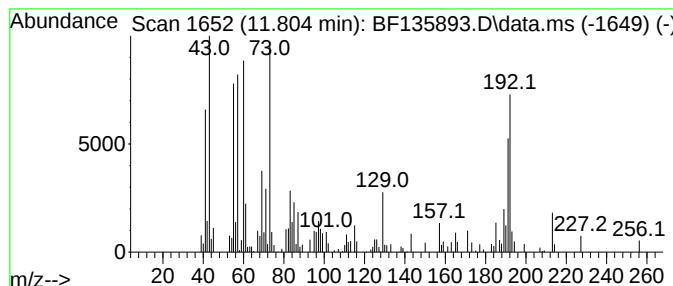
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	4.82 ng	100408	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tridecanoic acid	214	C13H26O2	000638-53-9	78
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	46
4			Undecanoic acid	186	C11H22O2	000112-37-8	46
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	46



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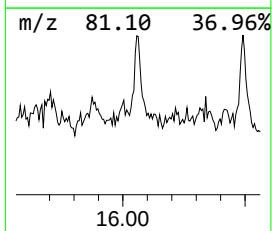
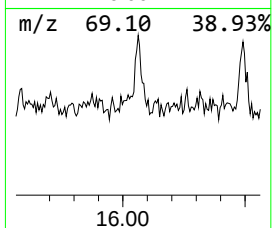
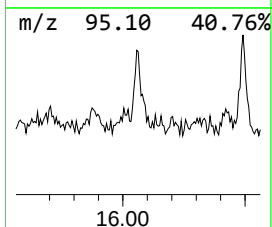
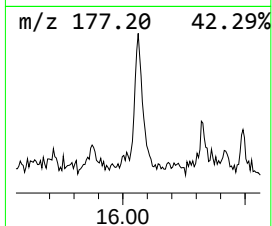
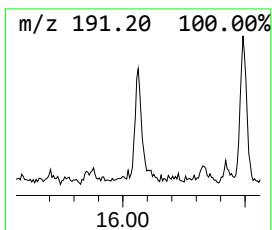
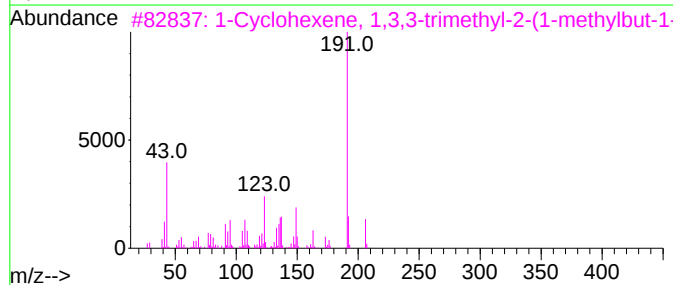
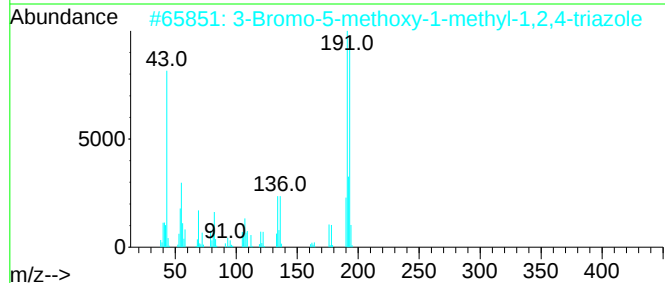
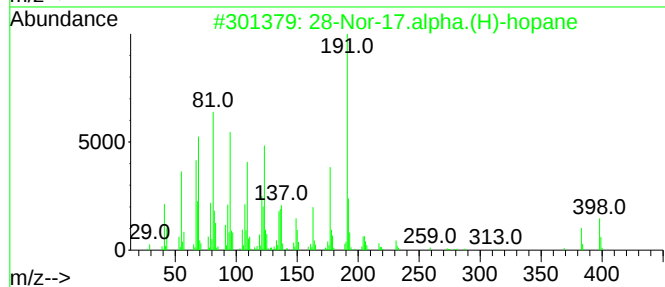
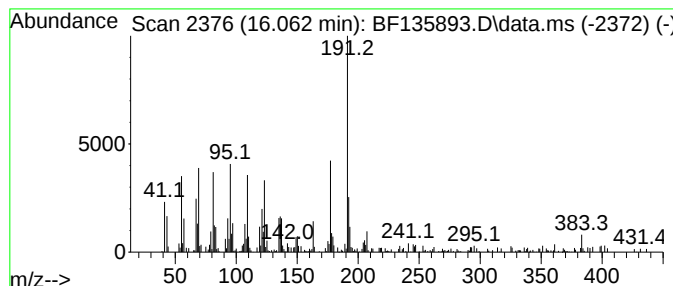
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 28-Nor-17.alpha.(H)-hopane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.062	15.55 ng	181781	Perylene-d12		15.415	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	28-Nor-17.alpha.(H)-hopane		398	C29H50	053584-60-4	90
2	3-Bromo-5-methoxy-1-methyl-1,2,4...		191	C4H6BrN3O	1000435-10-2	38
3	1-Cyclohexene, 1,3,3-trimethyl-2...		206	C14H22O	1000197-08-4	38
4	3-Fluoro-5-trifluoromethylbenzoi...		376	C20H28F4O2	1010338-65-7	27
5	.beta.-iso-Methyl ionone		206	C14H22O	1000285-40-2	25



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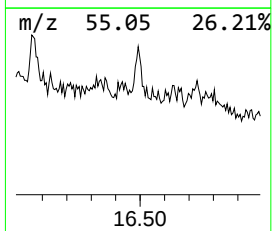
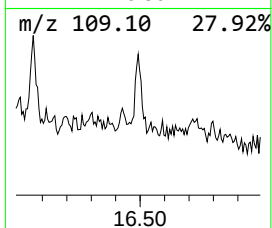
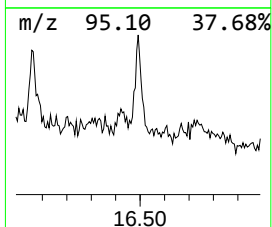
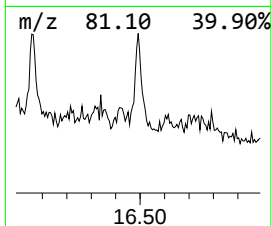
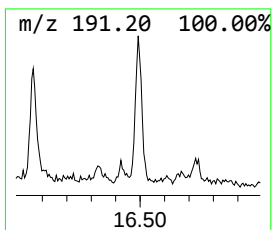
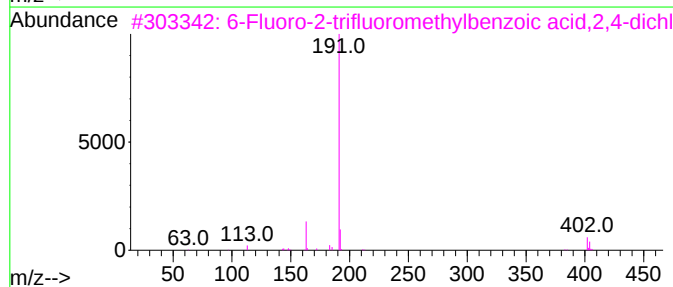
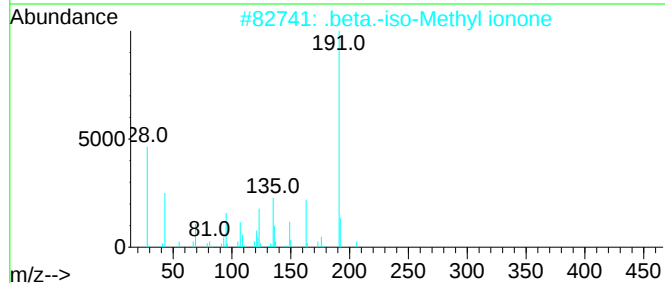
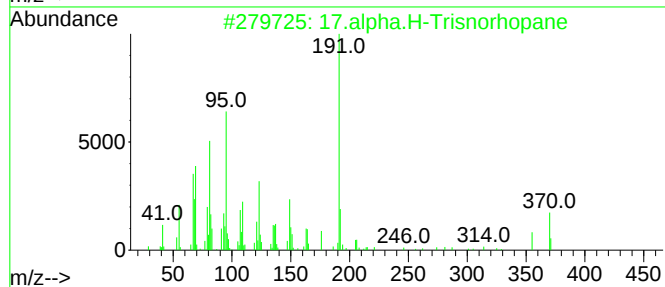
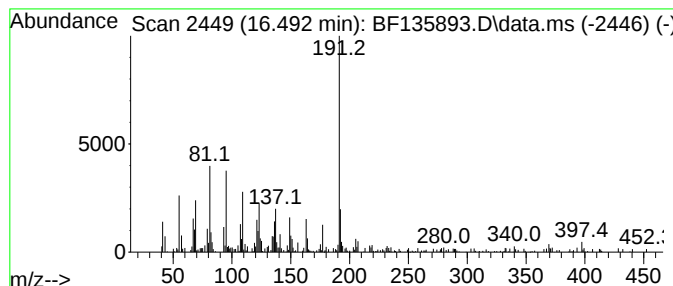
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 17.alpha.H-Trisnorhopane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.492	17.31 ng	202437	Perylene-d12	15.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17.alpha.H-Trisnorhopane	370	C27H46	053584-59-1	89
2			.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	47
3			6-Fluoro-2-trifluoromethylbenzoi...	402	C18H8Cl2F4O2	1010343-74-7	43
4			thiazolo[5,4-b]pyridin-2-amine, ...	191	C9H9N3S	1000400-23-3	38
5			2,3,4,5-Tetramethylacetanilide	191	C12H17NO	1000432-93-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101923\
Data File : BF135893.D
Acq On : 19 Oct 2023 18:46
Operator : CG\JU
Sample : 04907-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-03-101623

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.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
2-Pentanone, 4-...	4.939	13.2	ng	247798	1	6.734	376100	20.0
n-Hexadecanoic ...	11.804	4.8	ng	100408	4	11.269	416572	20.0
28-Nor-17.alpha...	16.062	15.6	ng	181781	6	15.415	233860	20.0
17.alpha.H-Tris...	16.492	17.3	ng	202437	6	15.415	233860	20.0