

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
 Data File : BF133885.D
 Acq On : 21 Jun 2023 22:47
 Operator : CG\JU
 Sample : 03289-19 2X
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-07-0-2.0

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: BF133885.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	15	rVB	176035	217732	34.61%	2.703%
2	2.240	21	26	32	rVB3	9653	14634	2.33%	0.182%
3	3.952	313	317	323	rVB2	6540	9148	1.45%	0.114%
4	5.081	506	509	517	rBV	137914	134566	21.39%	1.671%
5	5.487	574	578	591	rBV	684805	616074	97.92%	7.648%
6	5.881	642	645	654	rVB3	8235	8855	1.41%	0.110%
7	6.487	745	748	761	rBV	634553	595773	94.69%	7.396%
8	6.857	808	811	825	rVB	664211	569287	90.48%	7.067%
9	7.416	902	906	918	rBV	431215	362707	57.65%	4.503%
10	8.140	1025	1029	1035	rBV	736679	614402	97.65%	7.627%
11	9.210	1208	1211	1222	rBV	637737	582633	92.60%	7.233%
12	9.898	1324	1328	1331	rBV	603010	522730	83.08%	6.489%
13	9.928	1331	1333	1338	rVB3	7156	7972	1.27%	0.099%
14	10.610	1445	1449	1458	rBV	52735	43834	6.97%	0.544%
15	10.686	1458	1462	1470	rBV	372302	320070	50.87%	3.973%
16	11.386	1578	1581	1584	rBV	583795	547491	87.02%	6.797%
17	11.410	1584	1585	1592	rVV	85531	72089	11.46%	0.895%
18	11.463	1592	1594	1598	rVB	14425	13250	2.11%	0.164%
19	11.622	1617	1621	1625	rBV3	7616	11954	1.90%	0.148%
20	11.722	1635	1638	1641	rBV4	5462	8122	1.29%	0.101%
21	11.892	1664	1667	1669	rBV	19930	18464	2.93%	0.229%
22	11.922	1669	1672	1678	rVB3	56999	65446	10.40%	0.812%
23	12.004	1683	1686	1689	rVV2	30004	34821	5.53%	0.432%
24	12.028	1689	1690	1694	rVB	15742	12189	1.94%	0.151%
25	12.192	1715	1718	1720	rBV2	11488	11173	1.78%	0.139%
26	12.222	1720	1723	1725	rVB	13735	12861	2.04%	0.160%
27	12.451	1758	1762	1764	rBV	19697	21206	3.37%	0.263%
28	12.480	1765	1767	1770	rVV4	10622	11561	1.84%	0.144%
29	12.533	1773	1776	1781	rBV2	22011	23341	3.71%	0.290%
30	12.610	1785	1789	1793	rBV	251143	213355	33.91%	2.649%
31	12.710	1803	1806	1810	rBV6	14773	19178	3.05%	0.238%
32	12.839	1818	1828	1834	rBV	221508	252041	40.06%	3.129%
33	12.980	1849	1852	1860	rVB	640489	629172	100.00%	7.811%
34	13.057	1861	1865	1869	rBV3	23815	39183	6.23%	0.486%
35	13.145	1877	1880	1883	rBV5	18808	29539	4.69%	0.367%
36	13.169	1883	1884	1887	rVB	25315	15829	2.52%	0.197%

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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

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37	13.222	1890	1893	1894	rVV2	8028	7665	1.22%	0.095%
38	13.274	1898	1902	1905	rBV2	29574	28645	4.55%	0.356%
39	13.333	1910	1912	1916	rBV4	9890	10858	1.73%	0.135%
40	13.369	1916	1918	1921	rBV	22118	19247	3.06%	0.239%
41	13.398	1921	1923	1926	rBV3	14105	14020	2.23%	0.174%
42	13.563	1949	1951	1956	rVB5	11759	8819	1.40%	0.109%
43	13.686	1969	1972	1977	rBV	27490	28585	4.54%	0.355%
44	13.792	1988	1990	1992	rVB2	17336	14286	2.27%	0.177%
45	13.822	1993	1995	1997	rVB2	16783	10200	1.62%	0.127%
46	13.892	2004	2007	2013	rBV2	48053	60199	9.57%	0.747%
47	14.045	2029	2033	2036	rBV2	539829	577690	91.82%	7.172%
48	14.074	2036	2038	2047	rVB	95788	90042	14.31%	1.118%
49	14.916	2179	2181	2184	rVB	42023	31973	5.08%	0.397%
50	15.110	2211	2214	2222	rVB	65767	121810	19.36%	1.512%
51	15.492	2276	2279	2283	rVB	45973	50190	7.98%	0.623%
52	15.557	2286	2290	2294	rBV	241493	298305	47.41%	3.703%

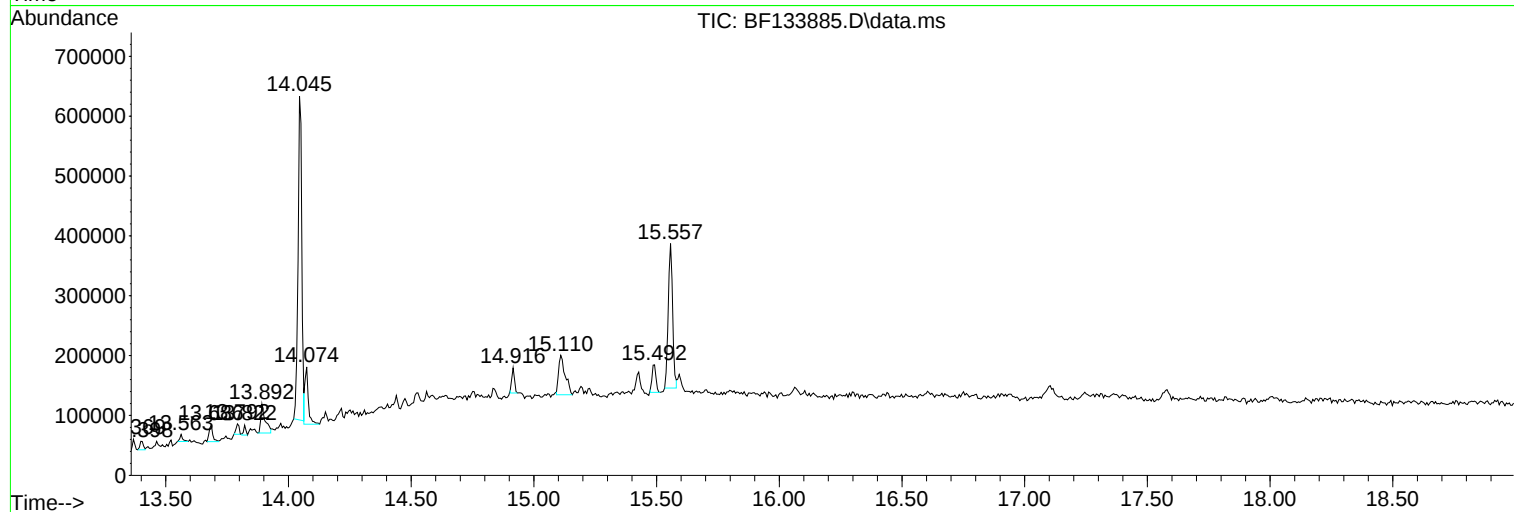
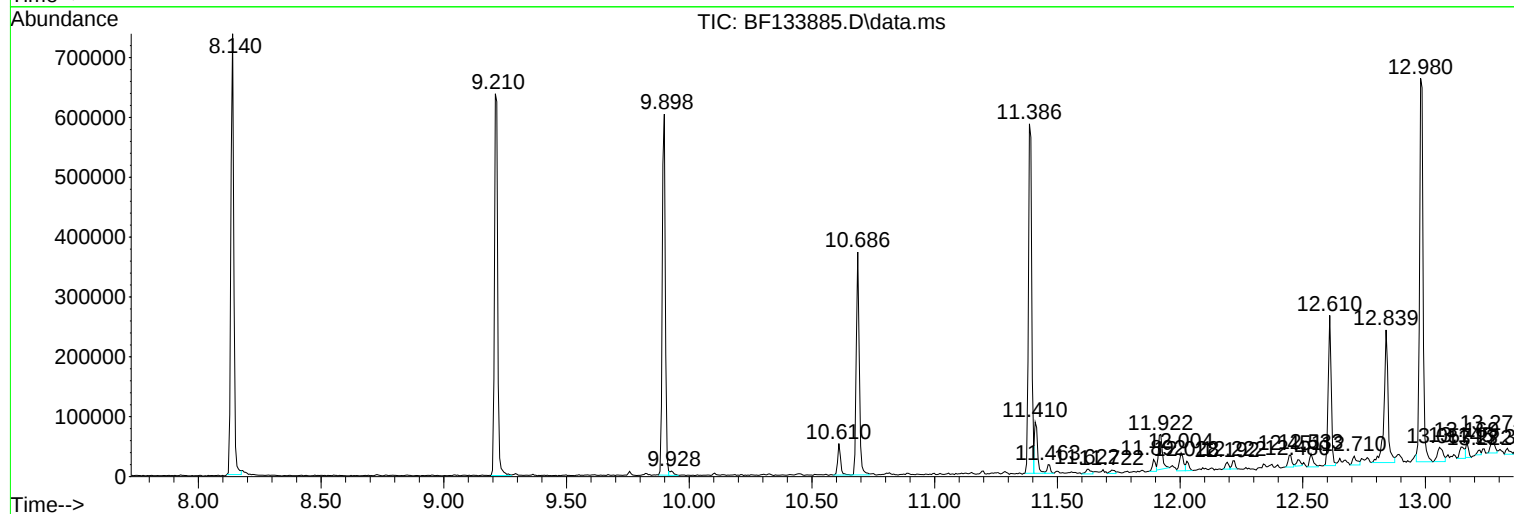
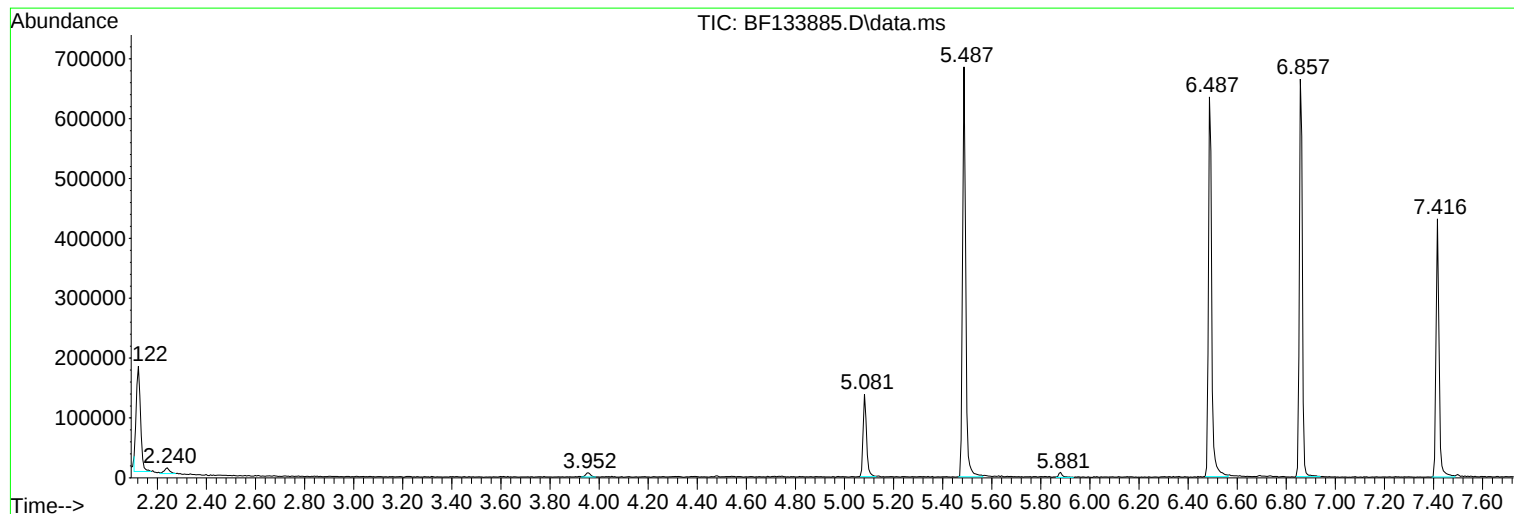
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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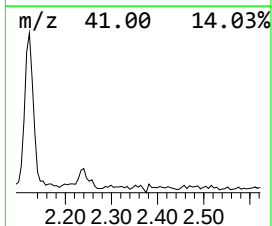
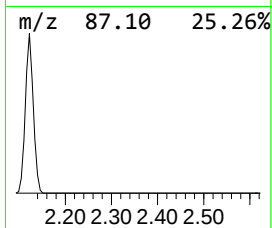
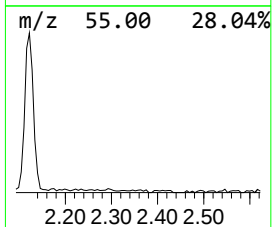
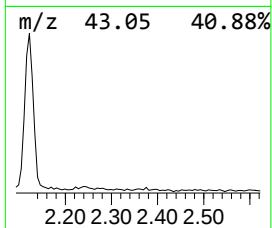
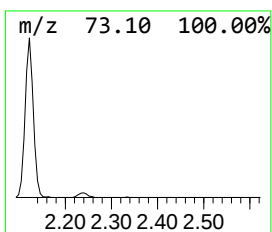
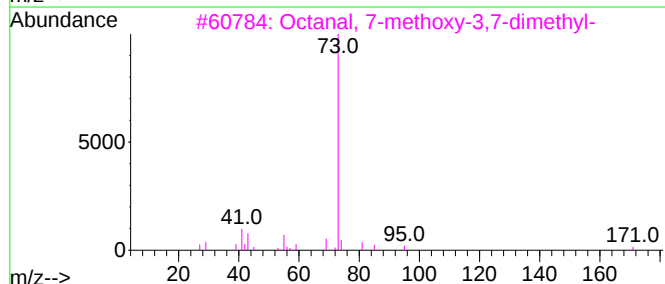
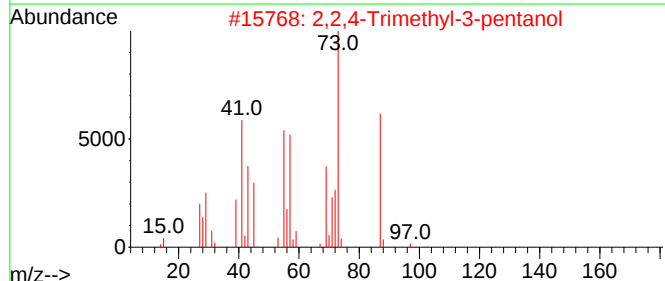
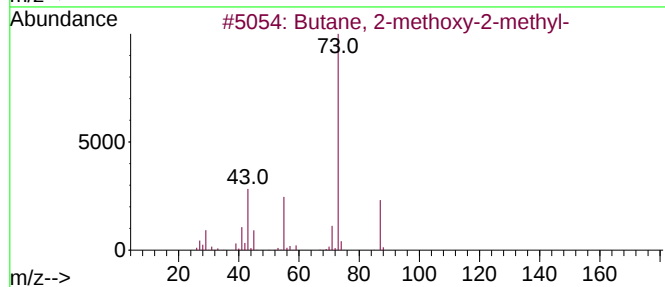
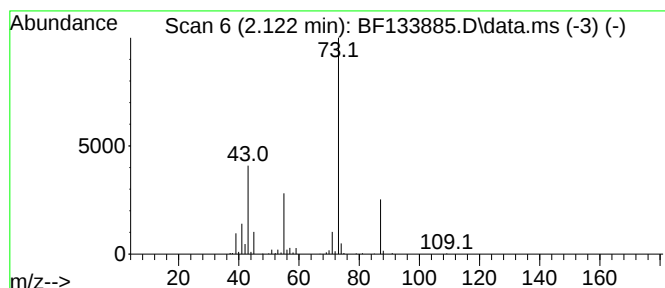
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	7.65 ng	217732	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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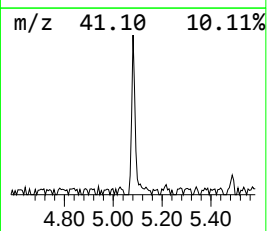
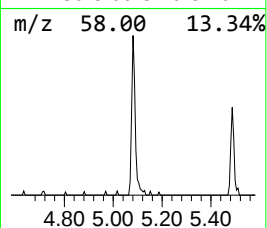
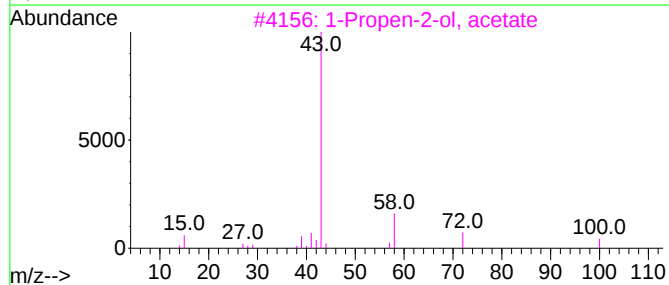
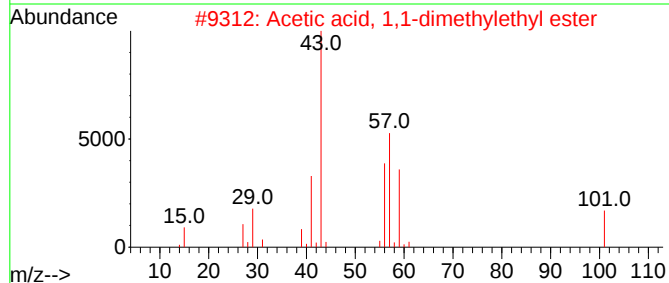
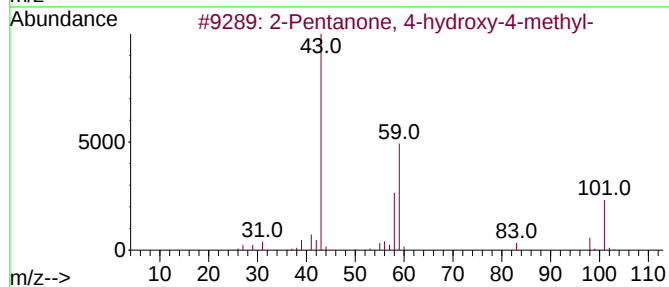
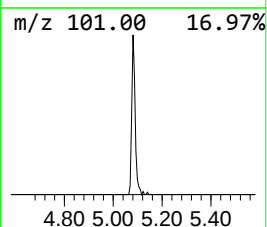
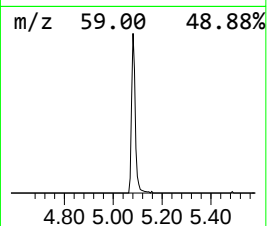
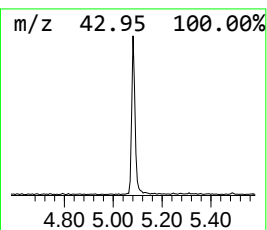
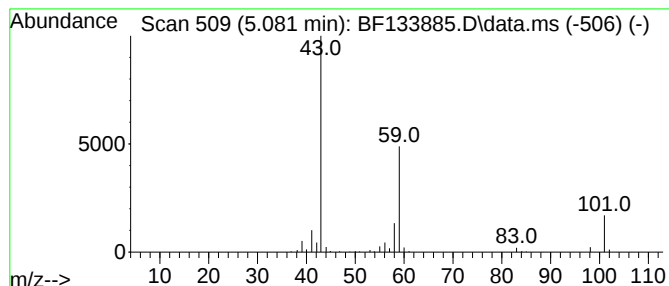
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	4.73 ng	134566	1,4-Dichlorobenzene-d4	6.857

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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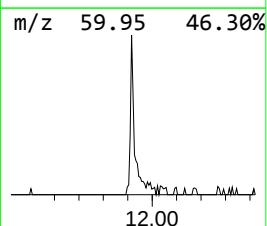
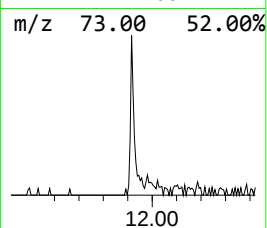
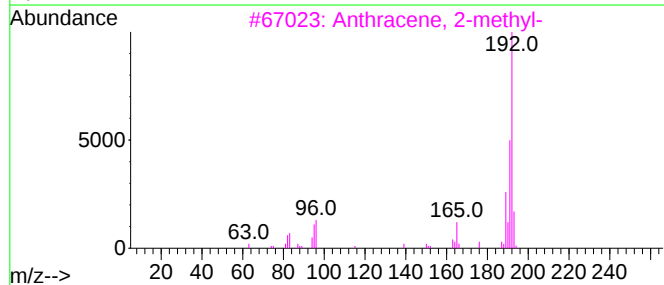
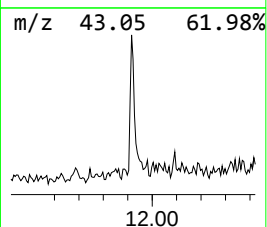
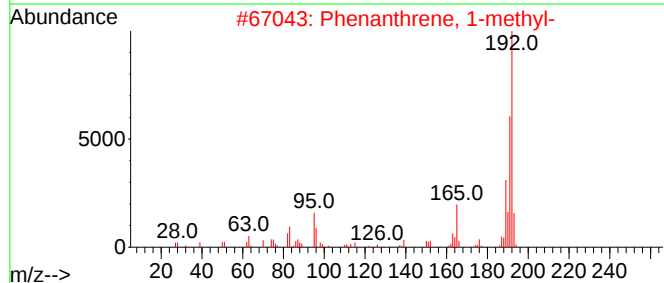
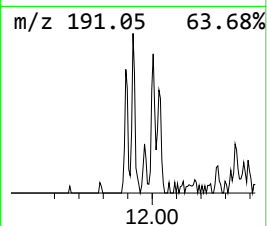
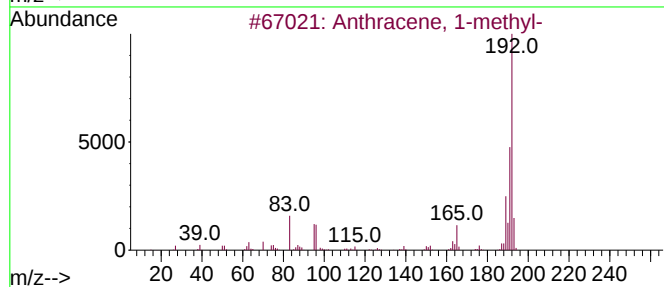
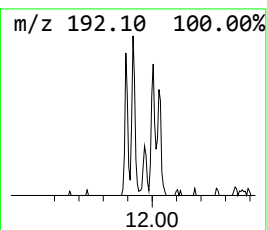
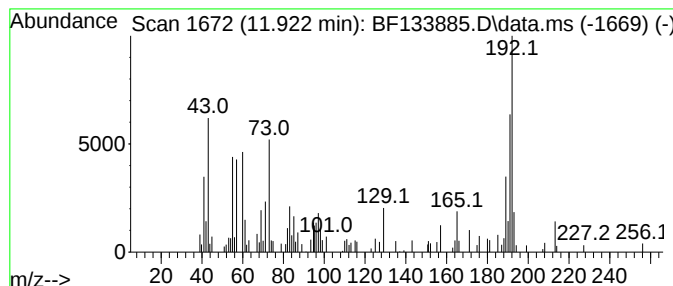
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Anthracene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	2.39 ng	65446	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 1-methyl-	192	C15H12	000610-48-0	78
2			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	70
3			Anthracene, 2-methyl-	192	C15H12	000613-12-7	58
4			Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	55
5			Anthracene, 9-methyl-	192	C15H12	000779-02-2	55



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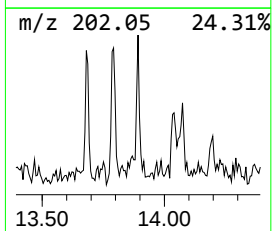
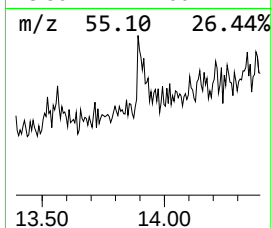
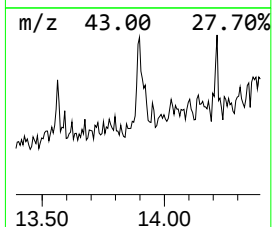
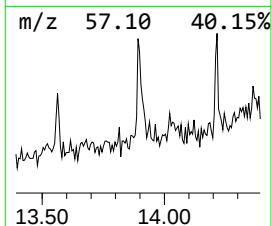
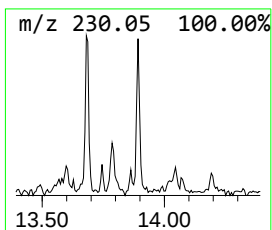
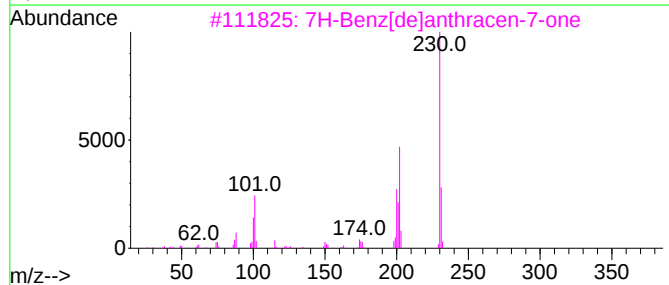
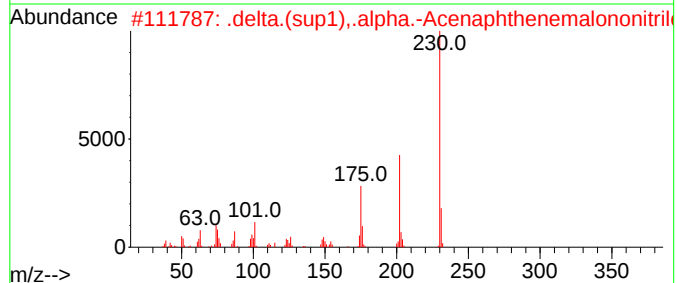
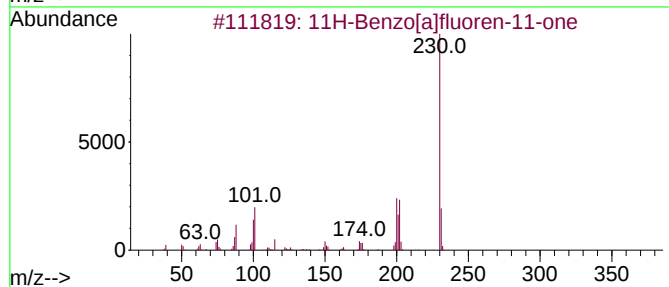
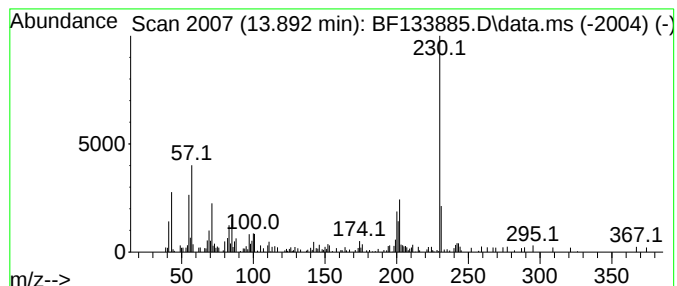
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 11H-Benzo[a]fluoren-11-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	2.08 ng	60199	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	86
2			.delta.(sup1),.alpha.-Acenaphthe...	230	C15H6N2O	014619-86-4	64
3			7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	59
4			1-Pyrenecarboxaldehyde	230	C17H10O	003029-19-4	53
5			2-Carbaldehyde-4-hydroxyquinolin...	287	C16H21N02Si	1000463-11-6	50



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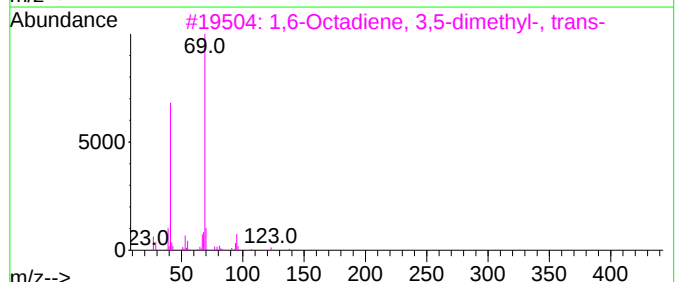
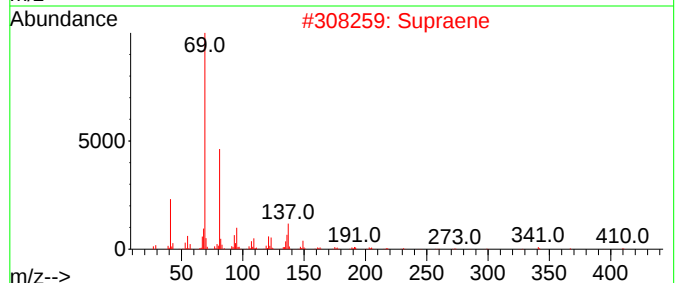
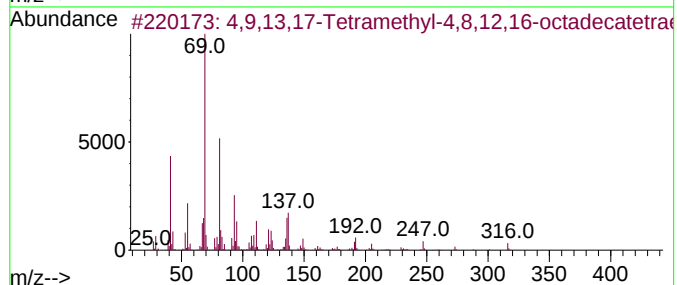
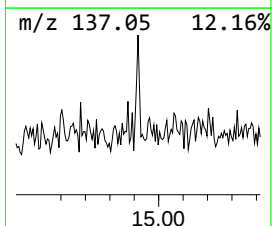
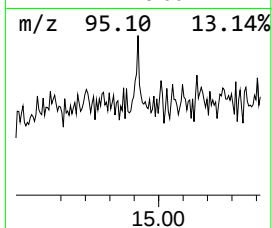
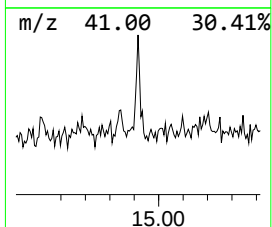
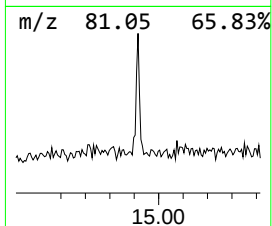
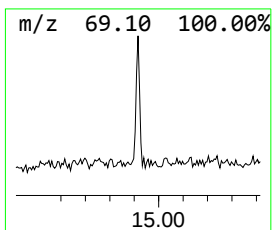
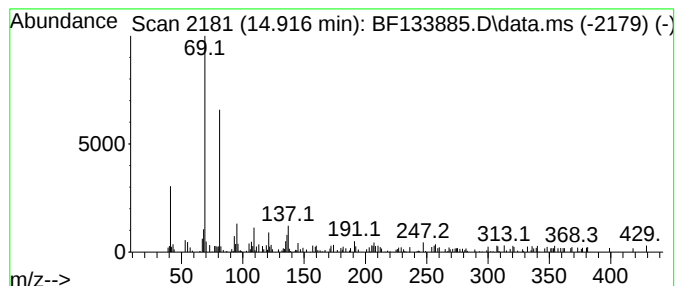
Instrument :
BNA_F
ClientSampleId :
SB-07-0-2.0

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 5 4,9,13,17-Tetramethyl-4,8,12,16-octadecatetraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.916	2.14 ng	31973	Perylene-d12	15.557	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	72
2	Supraene	410	C30H50	007683-64-9	64
3	1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	52
4	2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	50
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133885.D
Acq On : 21 Jun 2023 22:47
Operator : CG\JU
Sample : 03289-19 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-07-0-2.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.122	7.7	ng	217732	1	6.857	569287	20.0
2-Pentanone, 4-...	5.081	4.7	ng	134566	1	6.857	569287	20.0
Anthracene, 1-m...	11.922	2.4	ng	65446	4	11.392	547491	20.0
11H-Benzo[a]flu...	13.892	2.1	ng	60199	5	14.045	577690	20.0
4,9,13,17-Tetra...	14.916	2.1	ng	31973	6	15.557	298305	20.0