

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030823\
 Data File : BF132691.D
 Acq On : 08 Mar 2023 15:38
 Operator : CG\JU
 Sample : 01829-03
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS-03-20230306

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-BF022223.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132691.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.216	442	447	458	rVB	1107951	1204079	44.04%	4.437%
2	5.610	510	514	529	rBV	2568563	2400318	87.80%	8.844%
3	6.269	622	626	629	rBV	1826159	1676792	61.34%	6.178%
4	6.610	680	684	694	rBV	2559519	2403172	87.91%	8.855%
5	6.687	694	697	701	rVB	249357	198938	7.28%	0.733%
6	6.986	744	748	751	rBV	1192824	916826	33.54%	3.378%
7	7.551	840	844	847	rBV	1704072	1477535	54.05%	5.444%
8	8.269	963	966	972	rBV	1295998	1229684	44.98%	4.531%
9	9.345	1145	1149	1152	rBV	3357600	2733784	100.00%	10.073%
10	10.033	1262	1266	1269	rBV	1678474	1439768	52.67%	5.305%
11	10.427	1327	1333	1342	rBV3	30550	72343	2.65%	0.267%
12	10.745	1384	1387	1390	rVB	338477	260062	9.51%	0.958%
13	10.822	1397	1400	1404	rBV	1878204	1824076	66.72%	6.721%
14	11.169	1456	1459	1463	rVB4	34356	41775	1.53%	0.154%
15	11.527	1516	1520	1523	rBV	1740441	1444120	52.82%	5.321%
16	11.898	1580	1583	1587	rVB5	57358	69069	2.53%	0.254%
17	11.969	1593	1595	1598	rBV3	31185	34078	1.25%	0.126%
18	12.004	1598	1601	1603	rVV2	72149	85509	3.13%	0.315%
19	12.039	1603	1607	1622	rVB2	1021155	1274096	46.61%	4.695%
20	12.192	1631	1633	1635	rBV3	38742	32596	1.19%	0.120%
21	12.733	1723	1725	1726	rBV	46856	37393	1.37%	0.138%
22	12.827	1737	1741	1749	rBV	639122	713150	26.09%	2.628%
23	13.115	1786	1790	1794	rBV	2496162	2229315	81.55%	8.214%
24	13.486	1851	1853	1857	rBV	77148	60601	2.22%	0.223%
25	13.663	1880	1883	1892	rBV6	90677	163586	5.98%	0.603%
26	13.886	1918	1921	1927	rBV3	177632	220584	8.07%	0.813%
27	13.974	1933	1936	1939	rBV	242107	264260	9.67%	0.974%
28	14.004	1939	1941	1949	rVB	272808	340406	12.45%	1.254%
29	14.151	1963	1966	1969	rBV2	288211	293091	10.72%	1.080%
30	14.186	1969	1972	1976	rVB	1069371	940532	34.40%	3.466%
31	15.733	2231	2235	2243	rVB2	817620	1057968	38.70%	3.898%

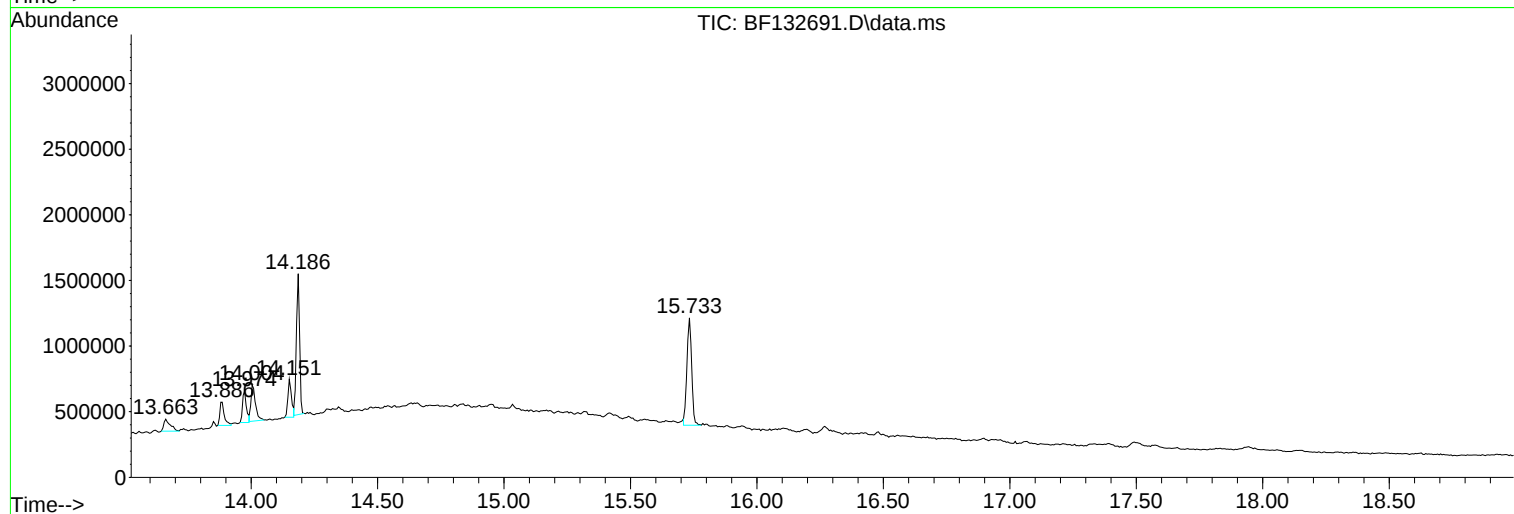
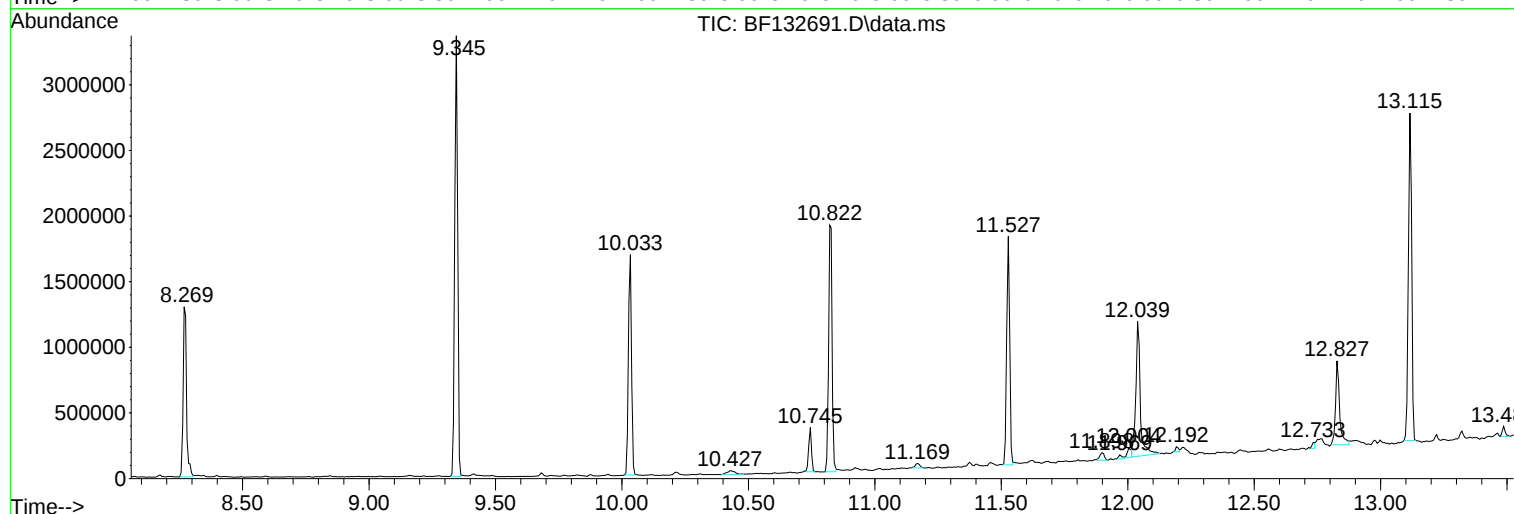
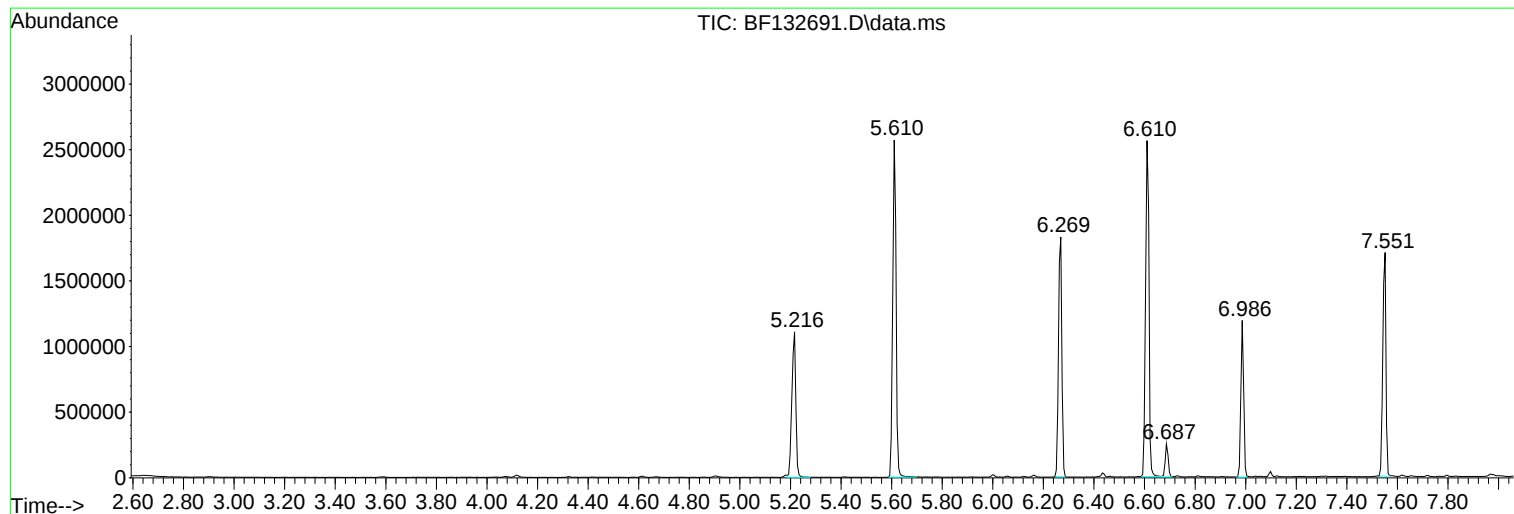
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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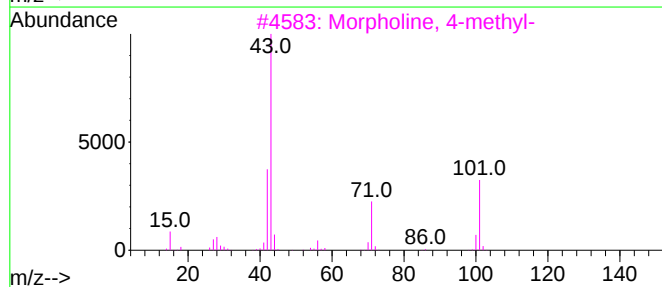
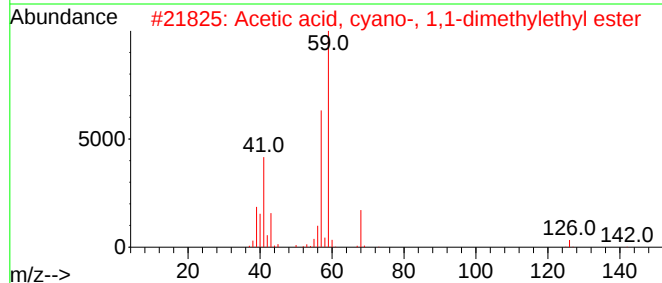
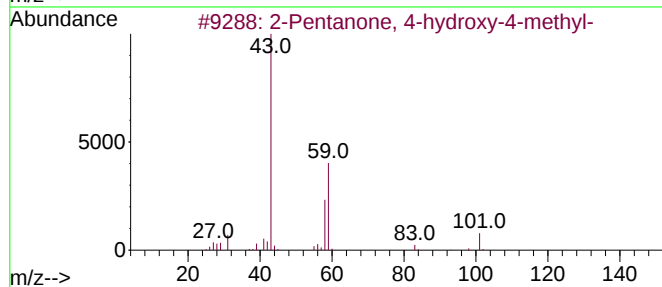
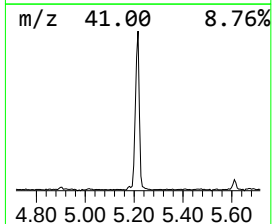
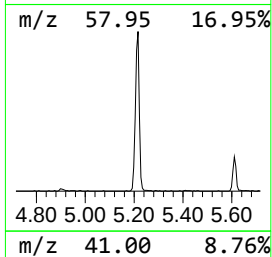
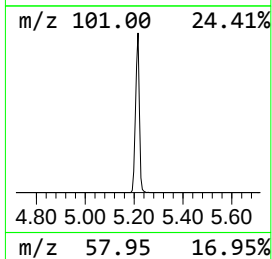
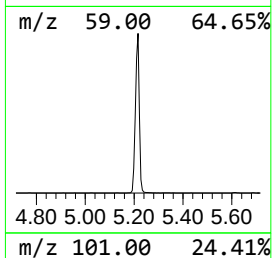
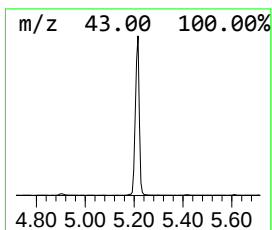
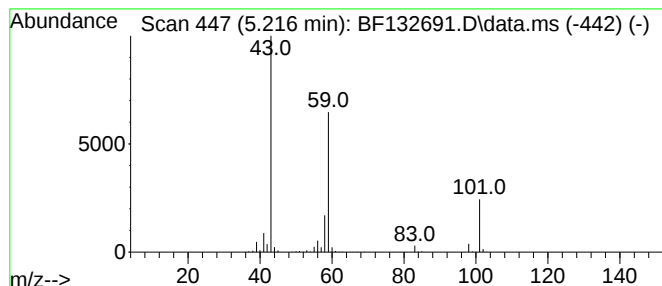
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.216	26.27 ng	1204080	1,4-Dichlorobenzene-d4	6.986

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			Acetone	58	C3H6O	000067-64-1	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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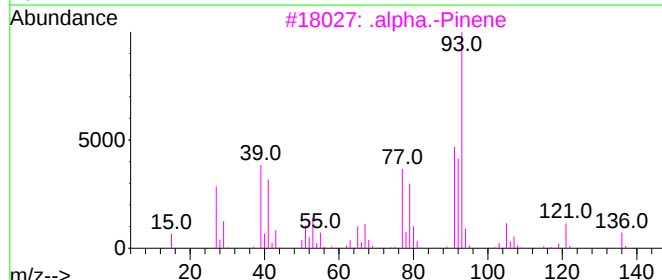
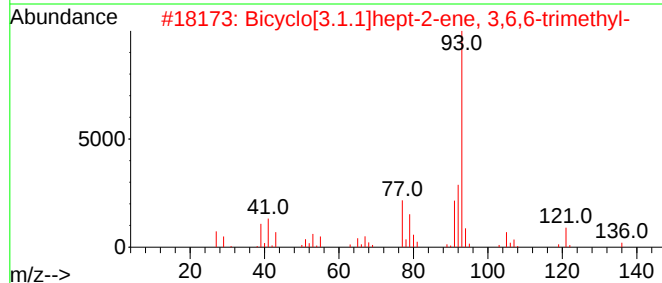
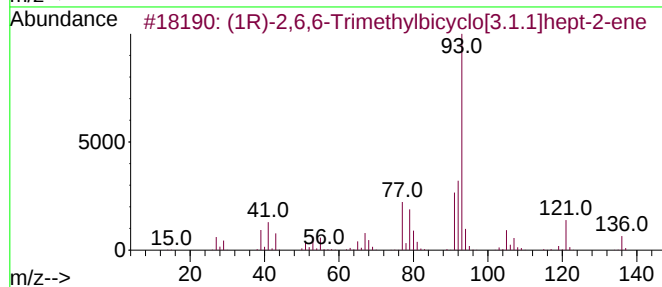
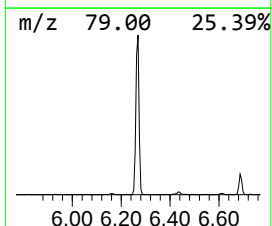
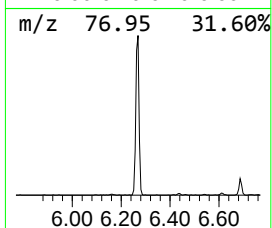
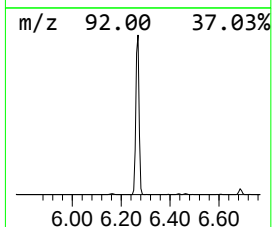
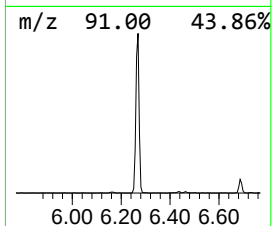
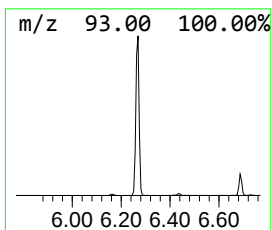
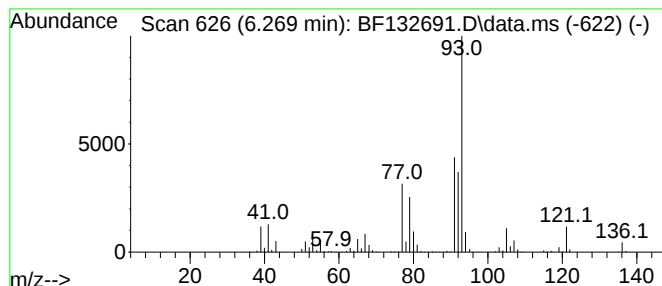
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 (1R)-2,6,6-Trimethylbicyclo... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.269	36.58 ng	1676790	1,4-Dichlorobenzene-d4	6.986

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-70-8	96
2		Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-	136	C10H16	004889-83-2	94
3		.alpha.-Pinene	136	C10H16	000080-56-8	94
4		(1S)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-26-4	91
5		3-Carene	136	C10H16	013466-78-9	91



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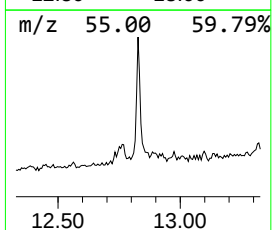
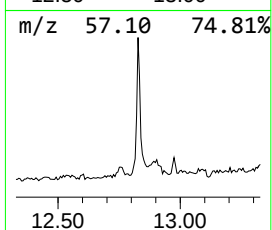
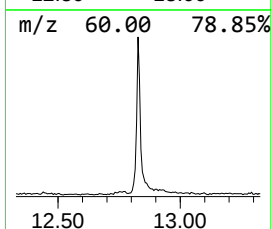
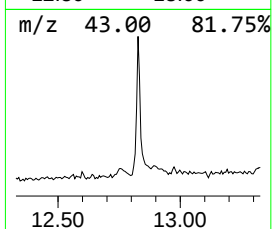
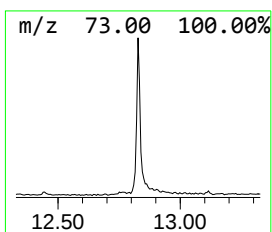
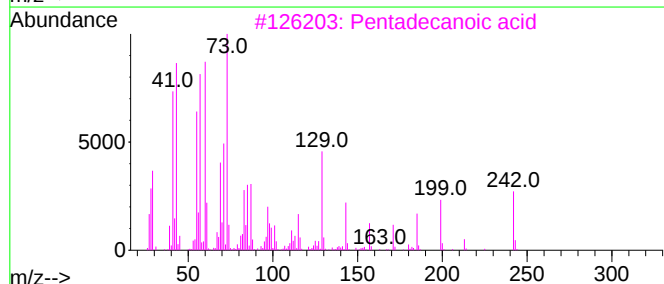
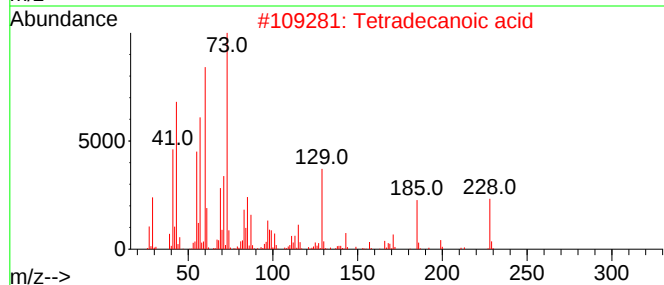
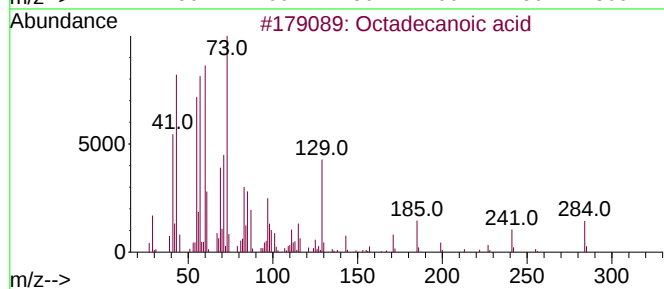
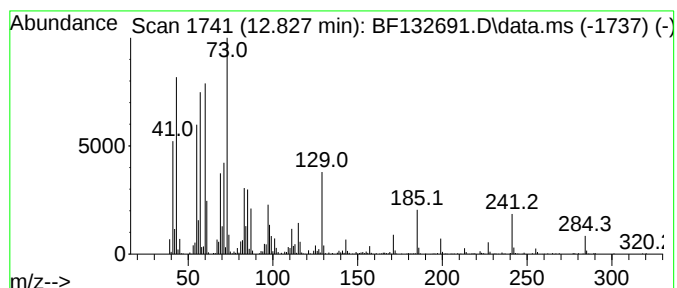
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.827	9.88 ng	713150	Phenanthrene-d10	11.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74



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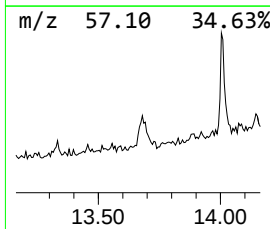
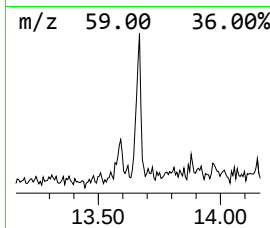
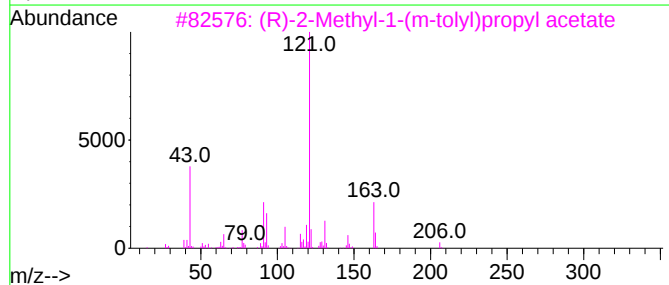
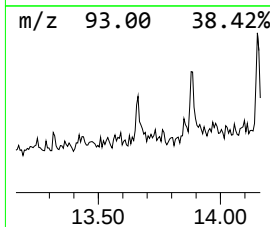
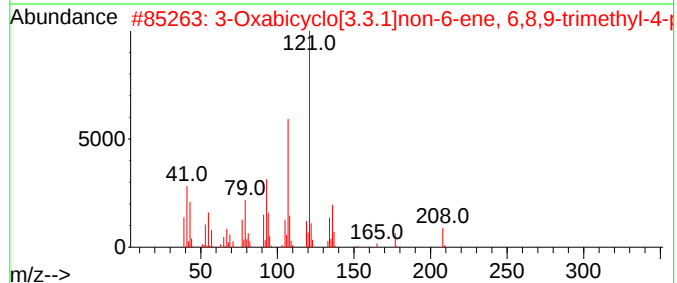
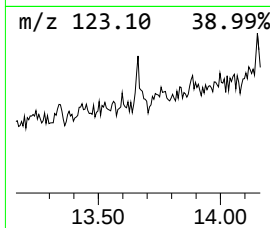
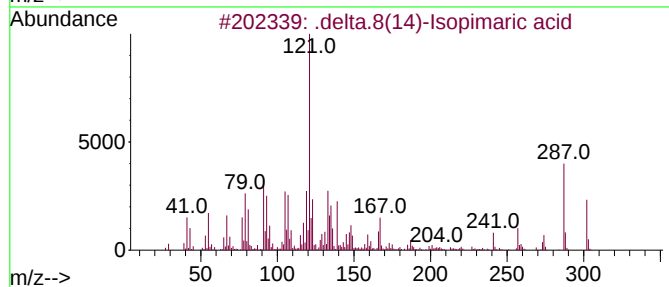
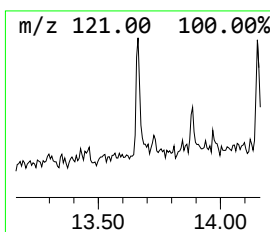
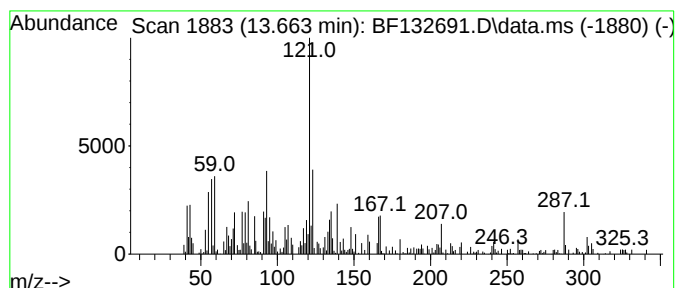
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Peak Number 4 .delta.8(14)-Isopimaric acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.663	3.48 ng	163586	Chrysene-d12	14.186

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.delta.8(14)-Isopimaric acid	302	C20H30O2	000471-74-9	60
2			3-Oxabicyclo[3.3.1]non-6-ene, 6,...	208	C14H24O	1000277-07-8	35
3			(R)-2-Methyl-1-(m-tolyl)propyl a...	206	C13H18O2	1396747-46-8	35
4			Formic acid, 2-isopropylphenyl e...	164	C10H12O2	1000368-95-8	27
5			Benzenamine, 3,4-dimethyl-	121	C8H11N	000095-64-7	22



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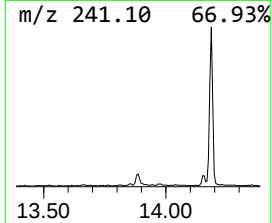
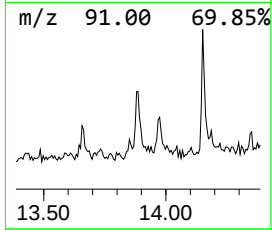
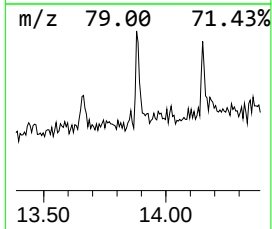
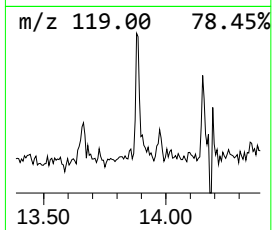
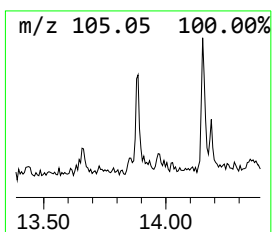
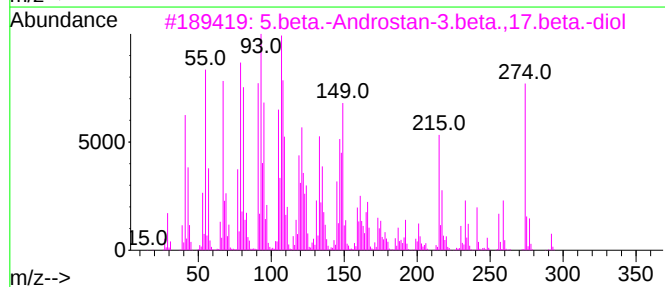
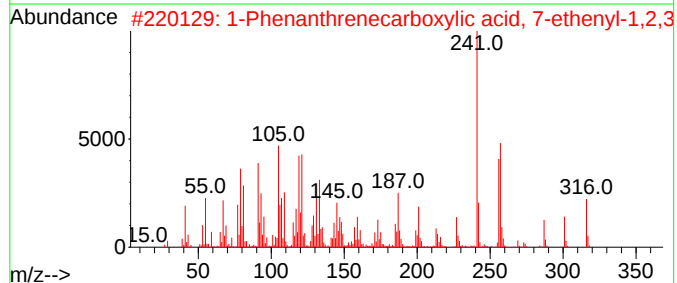
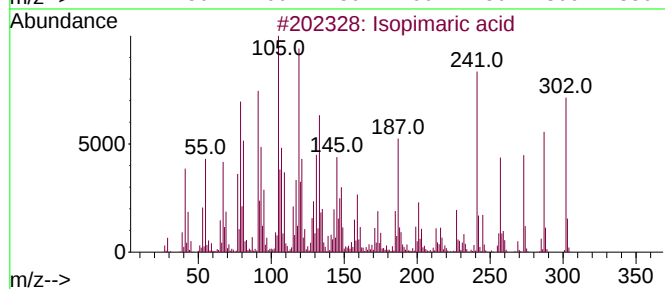
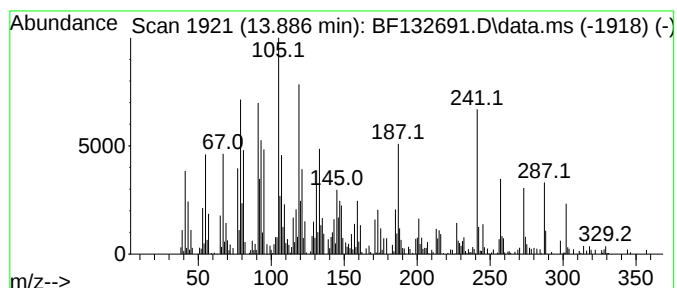
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Peak Number 5 Isopimaric acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	4.69 ng	220584	Chrysene-d12	14.186

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopimaric acid	302	C20H30O2	005835-26-7	93
2			1-Phenanthrenecarboxylic acid, 7...	316	C21H32O2	001686-62-0	90
3			5.beta.-Androstan-3.beta.,17.bet...	292	C19H32O2	006038-31-9	47
4			(1S,4aR,5S,8aR)-1,4a-Dimethyl-6-...	302	C20H30O2	002761-77-5	43
5			10,12-Tricosadiynoic acid, methy...	360	C24H40O2	1010333-59-4	38



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ClientSampleId :
SS-03-20230306

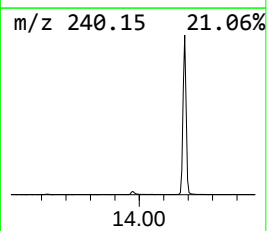
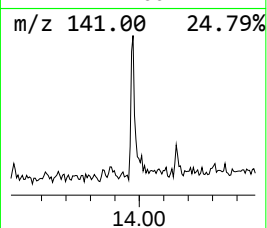
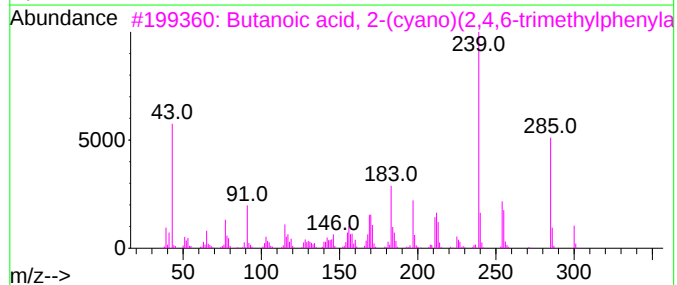
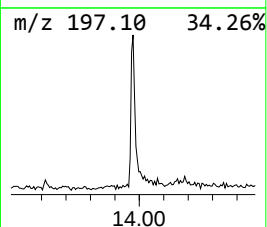
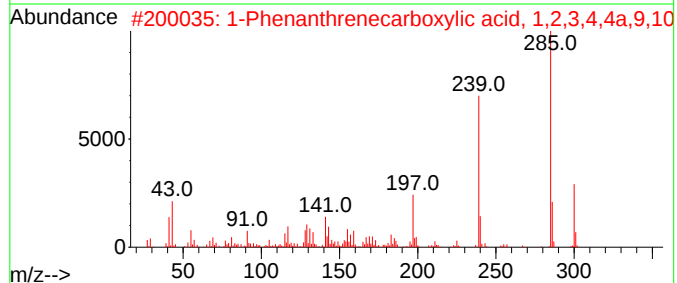
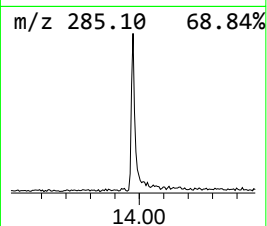
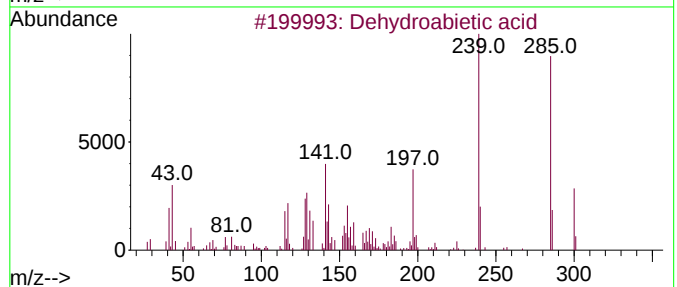
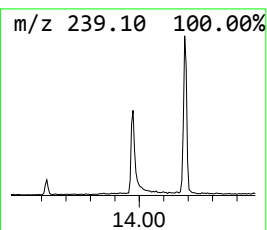
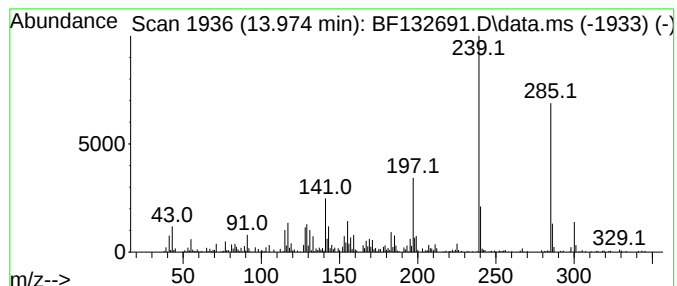
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Dehydroabiatic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.974	5.62 ng	264260	Chrysene-d12	14.186

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dehydroabiatic acid	300	C20H28O2	001740-19-8	98
2			1-Phenanthrenecarboxylic acid, 1...	300	C20H28O2	005155-70-4	95
3			Butanoic acid, 2-(cyano)(2,4,6-t...	300	C17H20N2O3	1000267-71-7	81
4			Ethyl 4-hydroxy-6-(trifluorometh...	285	C13H10F3NO3	026893-12-9	76
5			Kaura-9(11),16-dien-18-oic acid,...	300	C20H28O2	022338-67-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030823\
Data File : BF132691.D
Acq On : 08 Mar 2023 15:38
Operator : CG\JU
Sample : 01829-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

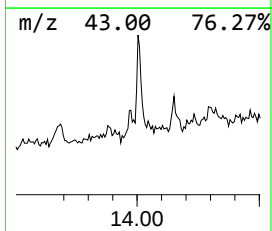
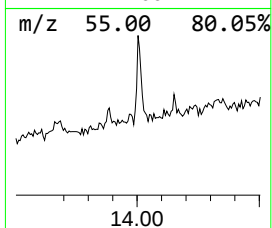
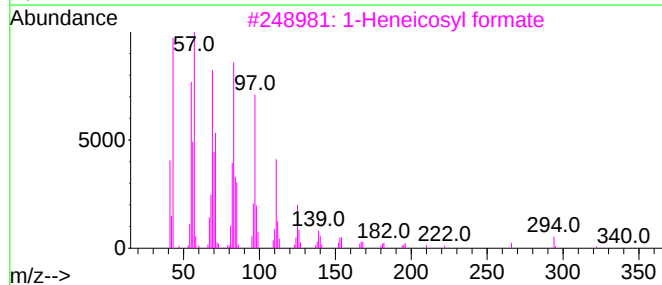
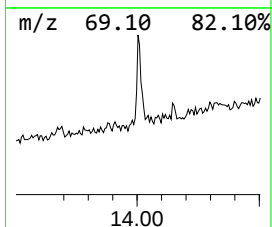
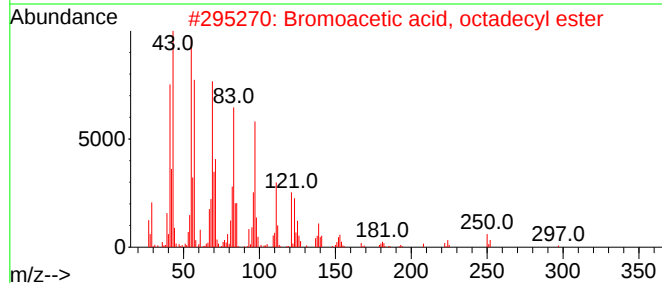
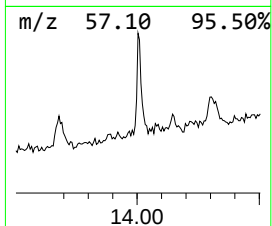
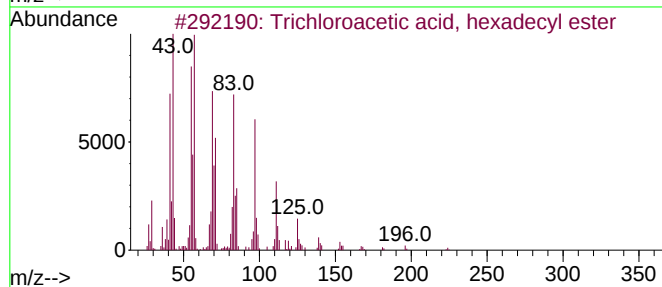
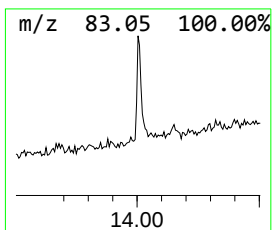
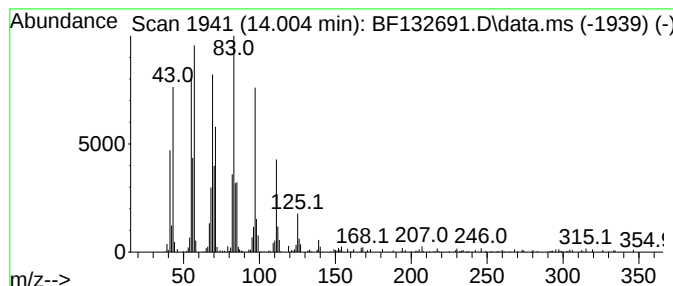
Instrument :
BNA_F
ClientSampleId :
SS-03-20230306

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.004	7.24 ng	340406	Chrysene-d12	14.186	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5	1-Nonadecene	266	C19H38	018435-45-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030823\
Data File : BF132691.D
Acq On : 08 Mar 2023 15:38
Operator : CG\JU
Sample : 01829-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-03-20230306

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.216	26.3	ng	1204080	1	6.986	916826	20.0
(1R)-2,6,6-Trim...	6.269	36.6	ng	1676790	1	6.986	916826	20.0
Octadecanoic acid	12.827	9.9	ng	713150	4	11.527	1444120	20.0
.delta.8(14)-Is...	13.663	3.5	ng	163586	5	14.186	940532	20.0
Isopimaric acid	13.886	4.7	ng	220584	5	14.186	940532	20.0
Dehydroabietic ...	13.974	5.6	ng	264260	5	14.186	940532	20.0
Trichloroacetic...	14.004	7.2	ng	340406	5	14.186	940532	20.0