

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031323\
 Data File : BF132760.D
 Acq On : 13 Mar 2023 15:08
 Operator : CG\JU
 Sample : 01853-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20230162-COMPOSITE-1

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: BF132760.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.598	338	342	348	rBV	54224	62013	1.30%	0.160%
2	5.204	439	445	460	rVB	1795646	2387377	50.17%	6.164%
3	5.604	509	513	528	rBV	4121496	3875887	81.46%	10.008%
4	5.987	574	578	582	rBV	96455	86878	1.83%	0.224%
5	6.604	678	683	686	rBV	3974269	3808381	80.04%	9.833%
6	6.969	742	745	749	rVB	1586350	1228722	25.82%	3.173%
7	7.533	837	841	844	rBV	2940530	2568029	53.97%	6.631%
8	8.251	960	963	967	rBV	1917129	1608229	33.80%	4.152%
9	9.327	1142	1146	1149	rBV	5617230	4600975	96.70%	11.880%
10	10.010	1259	1262	1266	rBV	2186015	1911591	40.17%	4.936%
11	10.198	1290	1294	1303	rBV5	33518	55289	1.16%	0.143%
12	10.727	1380	1384	1387	rVB	922778	825109	17.34%	2.130%
13	10.810	1393	1398	1401	rBV	3256960	3210903	67.48%	8.291%
14	11.504	1512	1516	1520	rBV	2265253	2056640	43.22%	5.310%
15	11.598	1529	1532	1535	rVB	73853	61450	1.29%	0.159%
16	12.016	1598	1603	1608	rBV	642387	652510	13.71%	1.685%
17	12.268	1643	1646	1649	rBV	68346	58670	1.23%	0.151%
18	12.727	1720	1724	1729	rBV	67966	76479	1.61%	0.197%
19	12.804	1733	1737	1749	rVB	128857	187784	3.95%	0.485%
20	12.957	1757	1763	1768	rBV3	84076	122540	2.58%	0.316%
21	13.098	1782	1787	1790	rBV	4710386	4758219	100.00%	12.286%
22	13.286	1816	1819	1821	rBV3	96289	108414	2.28%	0.280%
23	13.645	1876	1880	1883	rBV2	81444	107784	2.27%	0.278%
24	13.974	1933	1936	1947	rBV	637060	816224	17.15%	2.107%
25	14.115	1955	1960	1964	rBV2	47748	70281	1.48%	0.181%
26	14.162	1964	1968	1971	rBV	1386157	1317053	27.68%	3.401%
27	14.298	1987	1991	1996	rBV	87876	104587	2.20%	0.270%
28	14.604	2040	2043	2054	rBV2	120531	179381	3.77%	0.463%
29	14.921	2094	2097	2101	rVB	73002	77746	1.63%	0.201%
30	15.280	2154	2158	2162	rVB	93393	108137	2.27%	0.279%
31	15.692	2223	2228	2234	rBV2	978201	1253123	26.34%	3.236%
32	16.139	2302	2304	2310	rVB2	59667	81321	1.71%	0.210%
33	18.233	2656	2660	2674	rVB8	94900	301848	6.34%	0.779%

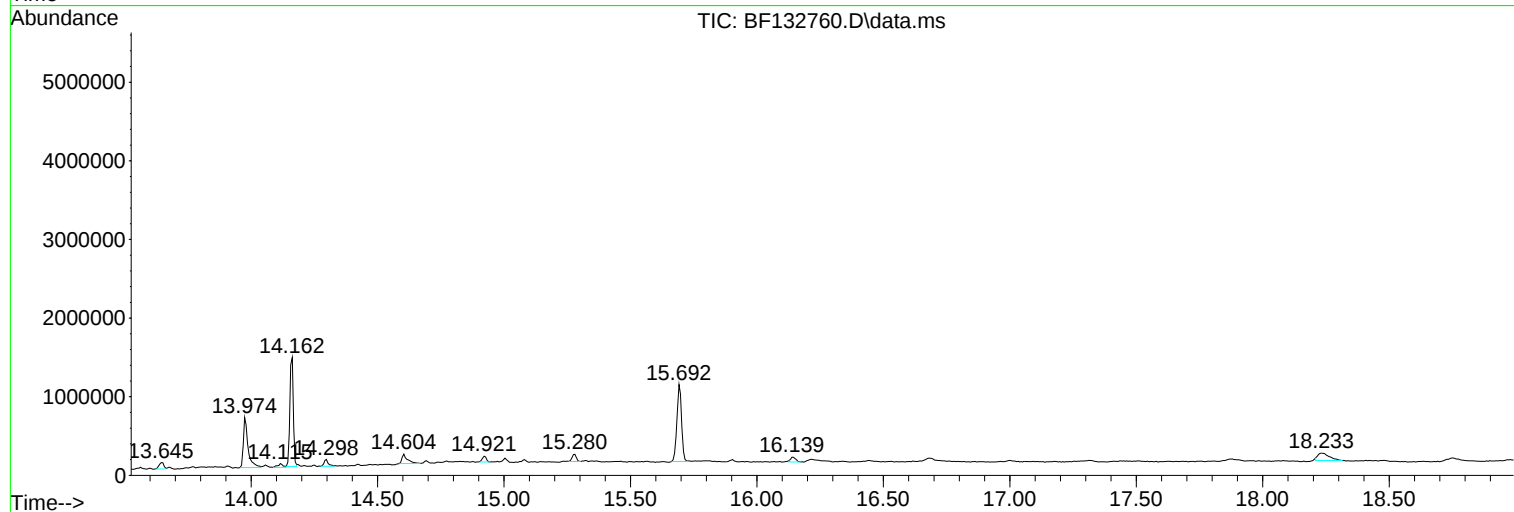
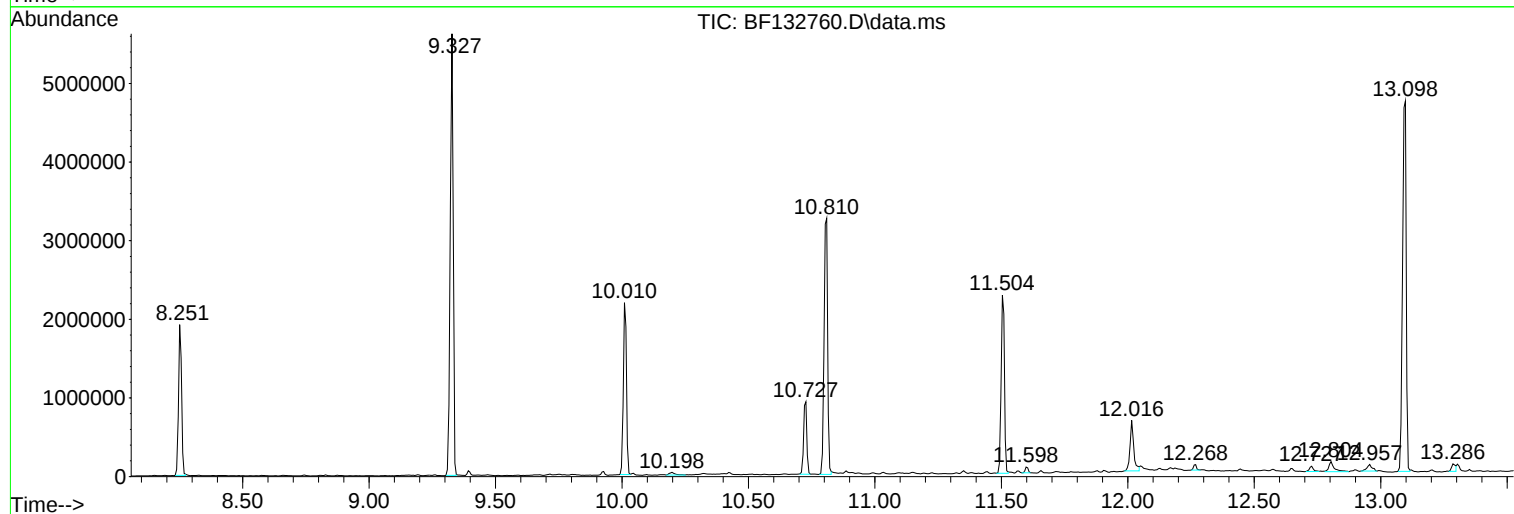
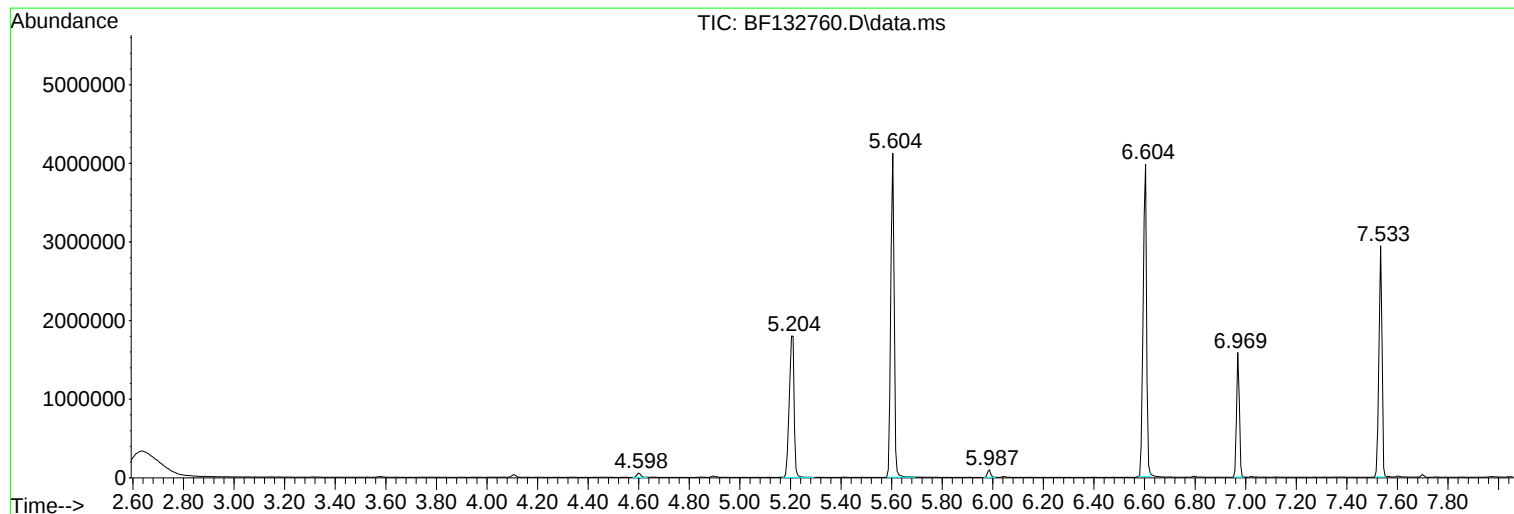
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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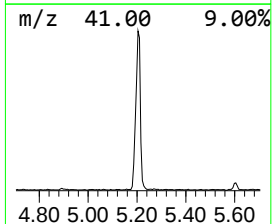
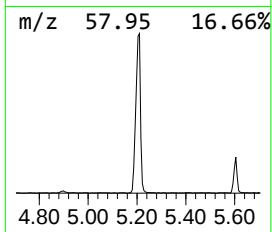
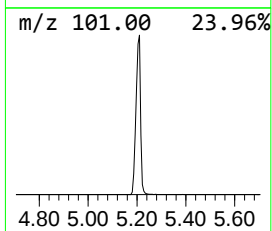
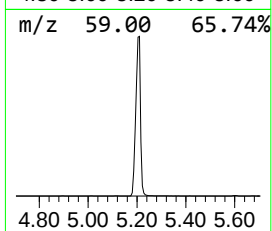
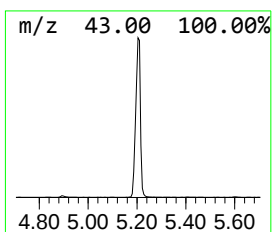
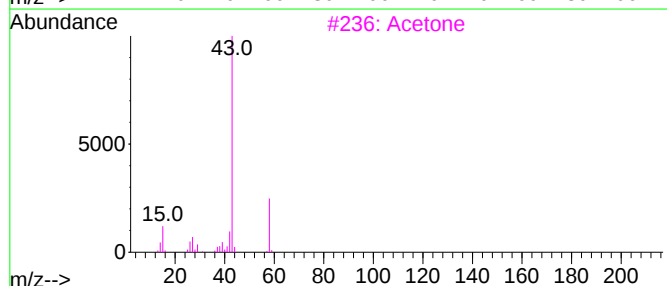
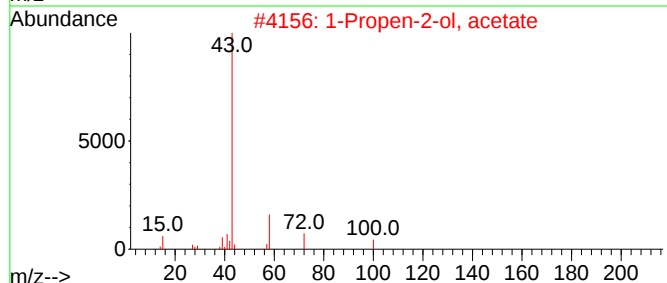
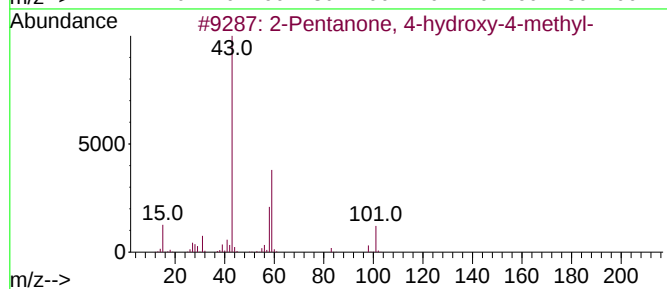
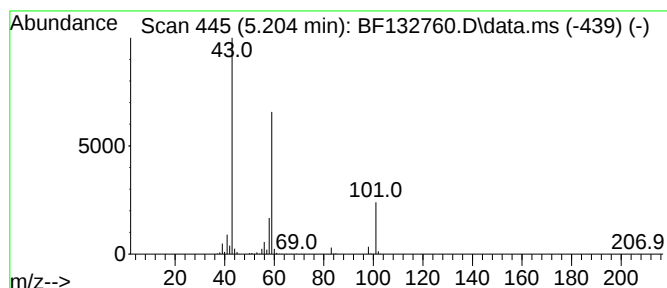
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.204	38.86 ng	2387380	1,4-Dichlorobenzene-d4	6.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3			Acetone	58	C3H6O	000067-64-1	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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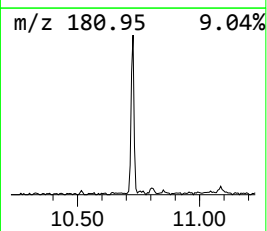
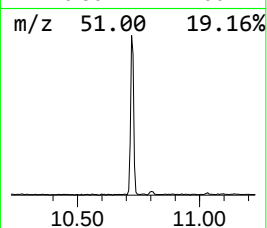
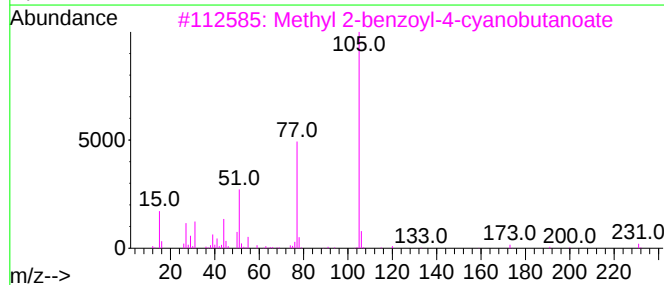
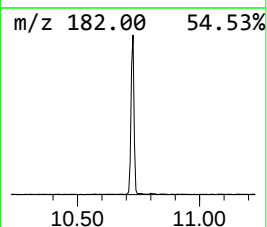
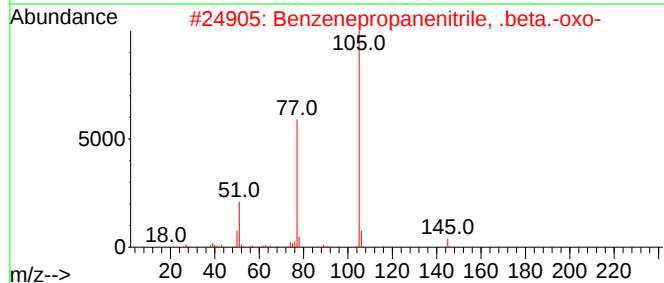
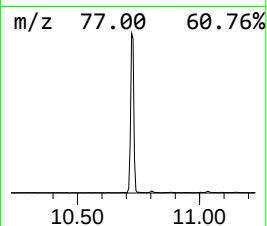
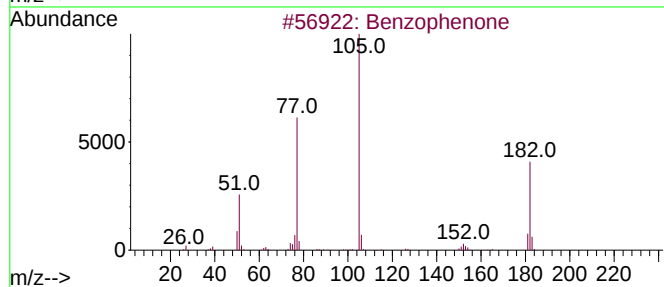
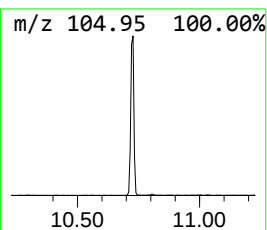
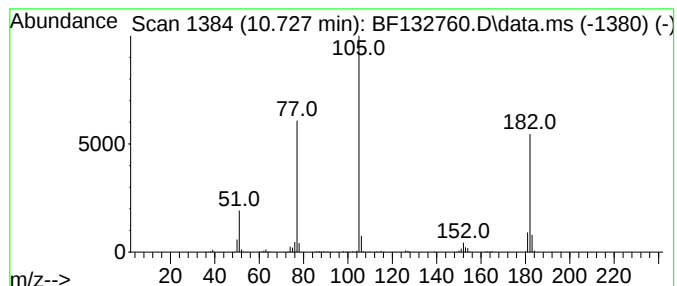
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Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.727	8.63 ng	825109	Acenaphthene-d10	10.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
3			Methyl 2-benzoyl-4-cyanobutanoate	231	C13H13NO3	1010486-83-8	47
4			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
5			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47



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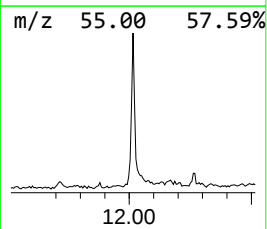
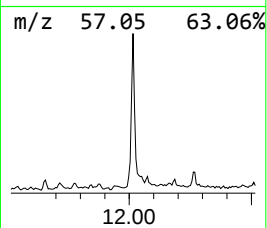
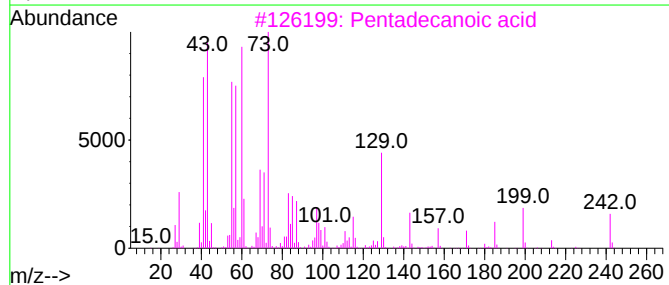
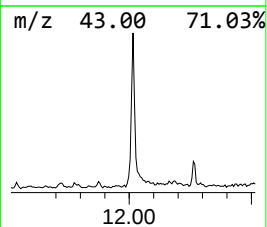
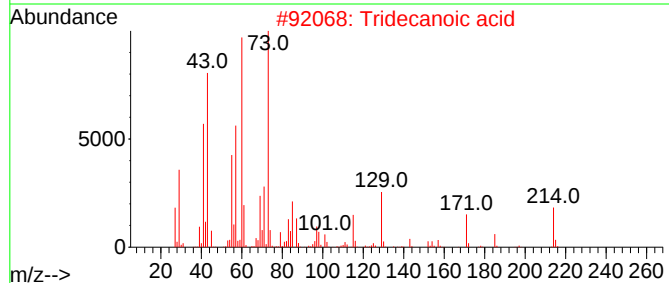
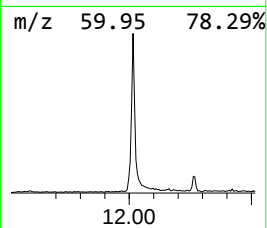
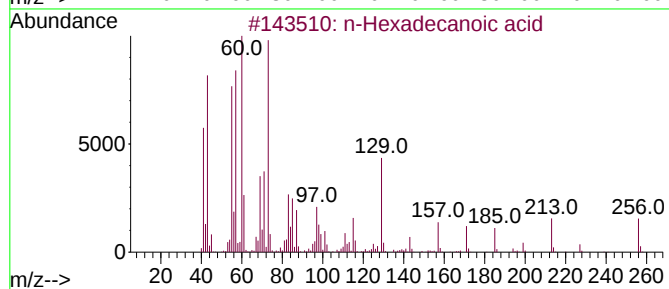
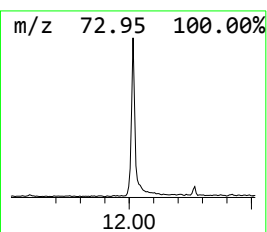
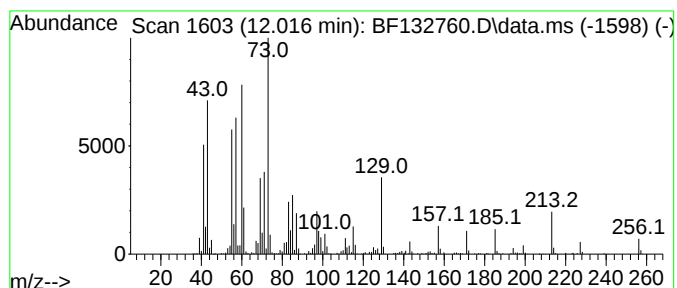
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.015	6.35 ng	652510	Phenanthrene-d10	11.504	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	47



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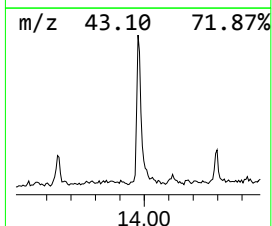
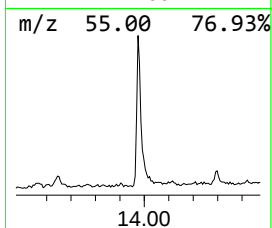
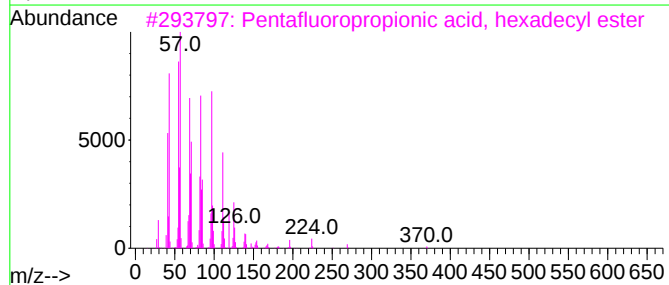
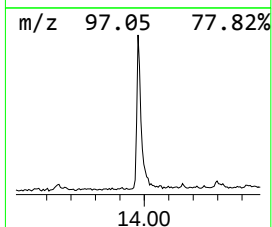
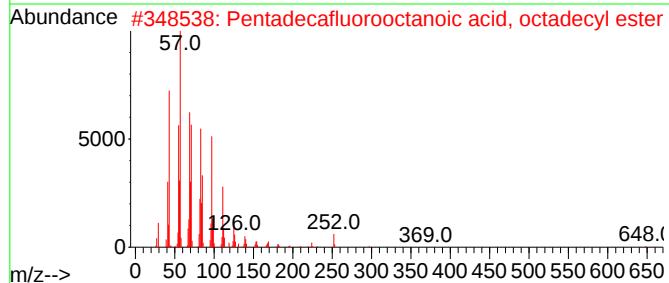
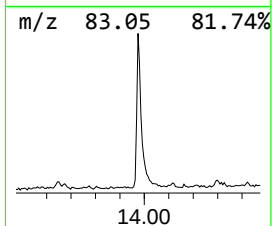
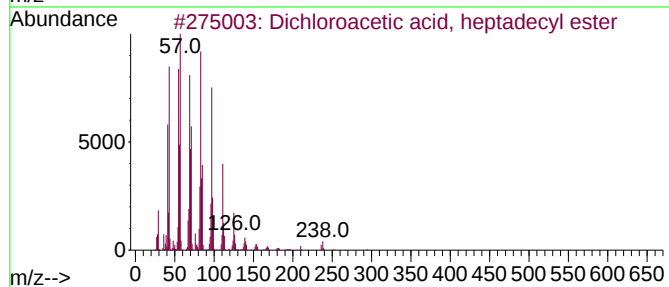
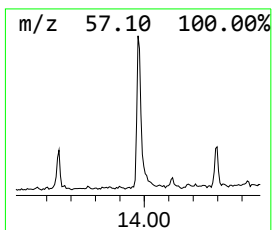
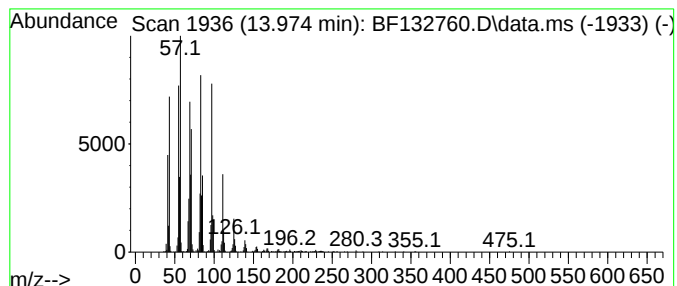
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Peak Number 4 Dichloroacetic acid, heptad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.974	12.39 ng	816224	Chrysene-d12	14.162

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
3			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
4			1-Hexacosene	364	C26H52	018835-33-1	91
5			5-Eicosene, (E)-	280	C20H40	074685-30-6	91



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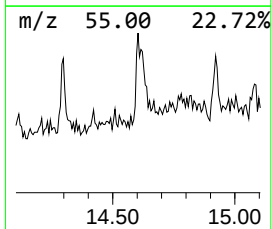
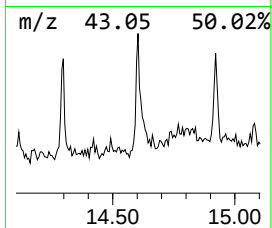
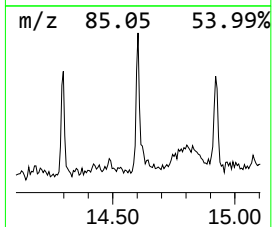
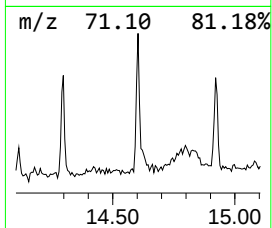
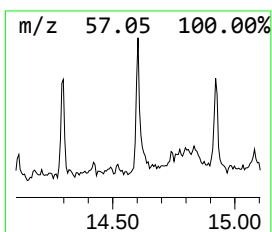
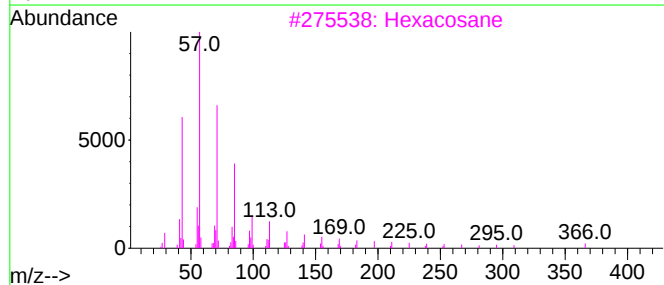
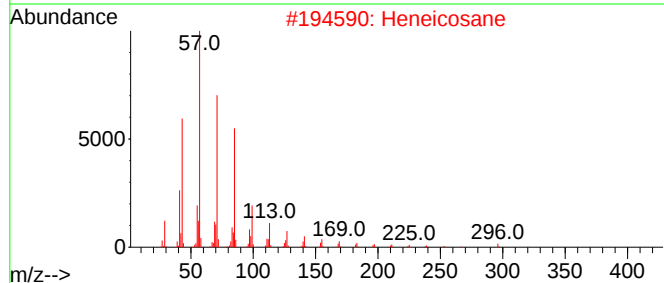
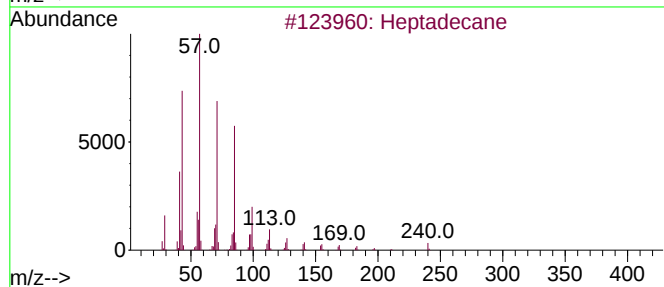
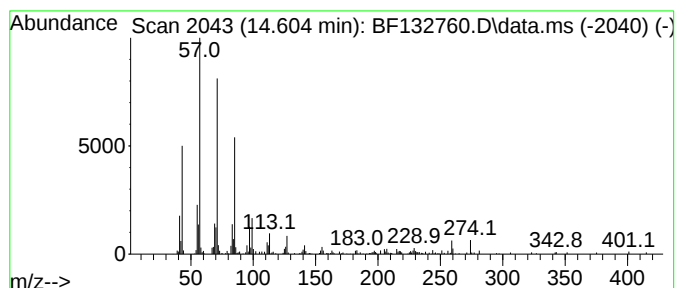
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Peak Number 5 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.604	2.72 ng	179381	Chrysene-d12	14.162

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	90
2			Heneicosane	296	C21H44	000629-94-7	90
3			Hexacosane	366	C26H54	000630-01-3	87
4			Tetradecane	198	C14H30	000629-59-4	87
5			Octacosane	394	C28H58	000630-02-4	87



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ClientSampleId :
20230162-COMPOSITE-1

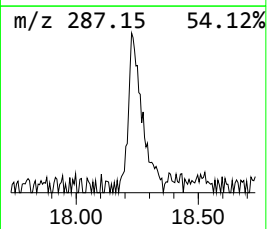
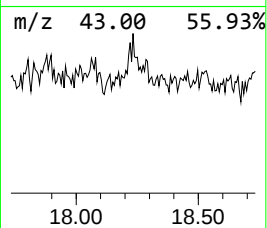
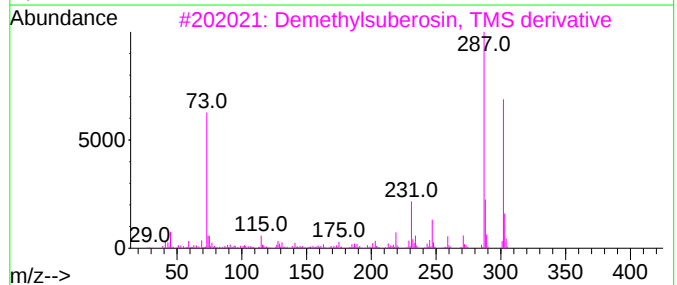
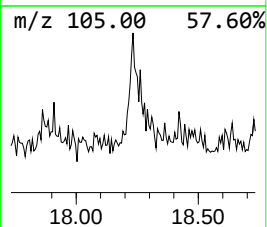
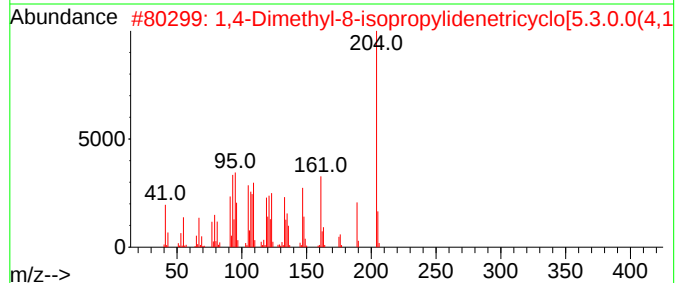
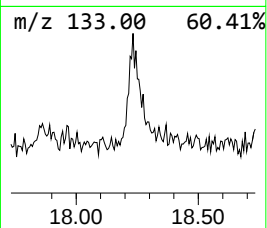
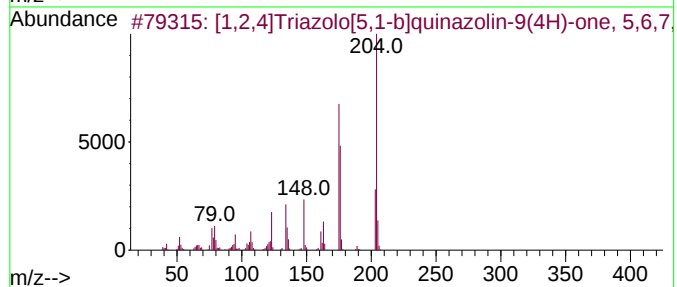
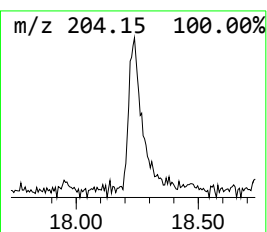
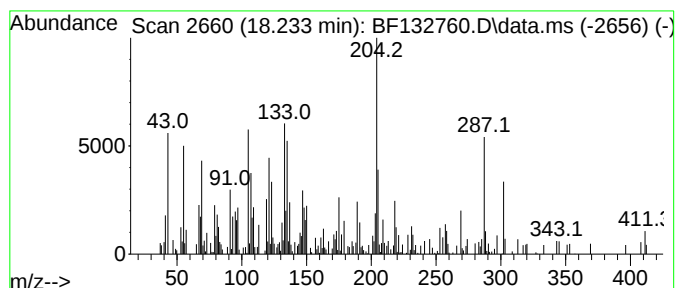
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown18.233 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.233	4.82 ng	301848	Perylene-d12	15.692

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	[1,2,4]Triazolo[5,1-b]quinazolin...	204	C10H12N4O	1000337-56-5	30		
2	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1010140-07-7	27		
3	Demethylsuberosin, TMS derivative	302	C17H22O3Si	1000480-22-8	25		
4	2-Methyl-3-n-heptyl-6-methoxy-1...	288	C17H24N2O2	1000250-74-6	22		
5	[1,1'-Biphenyl]-2,2'-dicarbonitrile	204	C14H8N2	004341-02-0	22		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031323\
Data File : BF132760.D
Acq On : 13 Mar 2023 15:08
Operator : CG\JU
Sample : 01853-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20230162-COMPOSITE-1

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-...	5.204	38.9	ng	2387380	1	6.969	1228720	20.0
Benzophenone	10.727	8.6	ng	825109	3	10.010	1911590	20.0
n-Hexadecanoic ...	12.015	6.3	ng	652510	4	11.504	2056640	20.0
Dichloroacetic ...	13.974	12.4	ng	816224	5	14.162	1317050	20.0
Heptadecane	14.604	2.7	ng	179381	5	14.162	1317050	20.0
unknown18.233	18.233	4.8	ng	301848	6	15.692	1253120	20.0