

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052523\
 Data File : BG057558.D
 Acq On : 25 May 2023 14:59
 Operator : CG/JU
 Sample : 02920-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 280608

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_G\Methods\8270-BG042723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057558.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.384	307	314	320	rBV	20881	32973	2.37%	0.445%
2	5.872	391	397	411	rBV	332693	556344	40.03%	7.508%
3	7.499	667	674	689	rBV	372328	650941	46.83%	8.785%
4	8.351	813	819	828	rBV	89424	150543	10.83%	2.032%
5	9.531	1012	1020	1033	rVB	232328	420462	30.25%	5.674%
6	11.194	1296	1303	1314	rBV	115948	212615	15.30%	2.869%
7	13.597	1705	1712	1719	rBV	671620	1093120	78.65%	14.752%
8	13.755	1734	1739	1746	rBV3	23741	44807	3.22%	0.605%
9	14.384	1843	1846	1854	rBV2	75407	143578	10.33%	1.938%
10	14.701	1896	1900	1904	rBV5	112914	190950	13.74%	2.577%
11	14.795	1912	1916	1921	rVB3	209041	348022	25.04%	4.697%
12	14.971	1942	1946	1951	rVB2	285747	490086	35.26%	6.614%
13	15.747	2076	2078	2084	rVB3	213275	265691	19.12%	3.586%
14	16.463	2196	2200	2205	rBV	465094	693395	49.89%	9.358%
15	20.287	2847	2851	2856	rVB	1089401	1389922	100.00%	18.758%
16	22.026	3144	3147	3156	rVB2	207710	359654	25.88%	4.854%
17	25.527	3736	3743	3755	rVB2	118701	366720	26.38%	4.949%

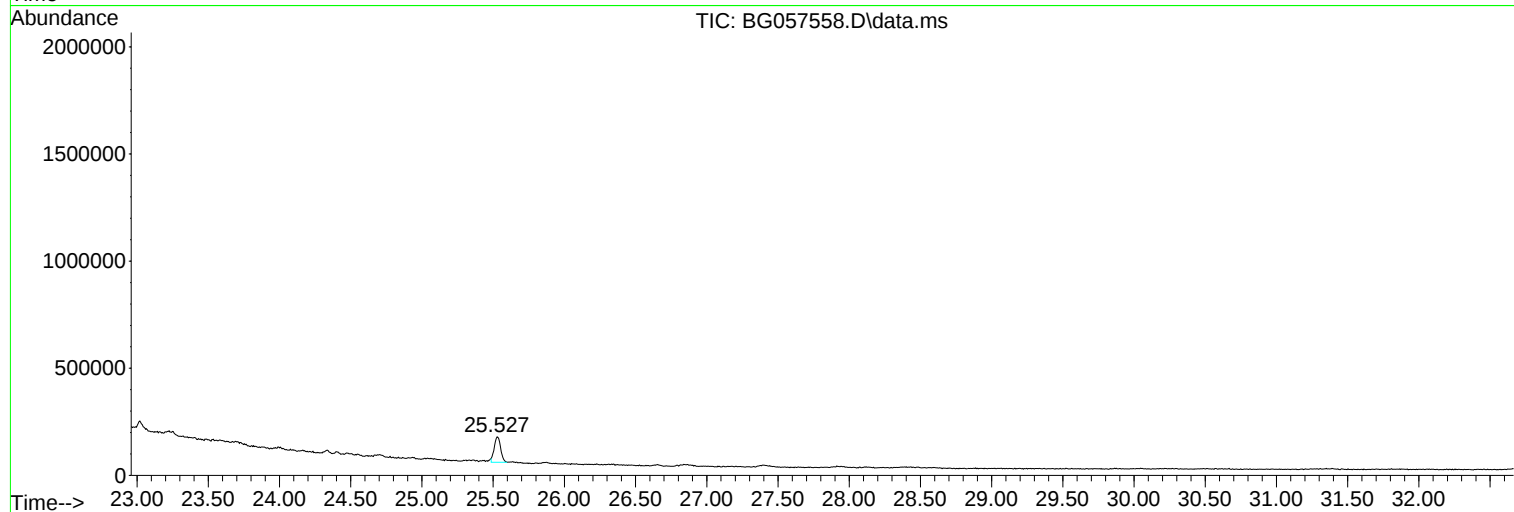
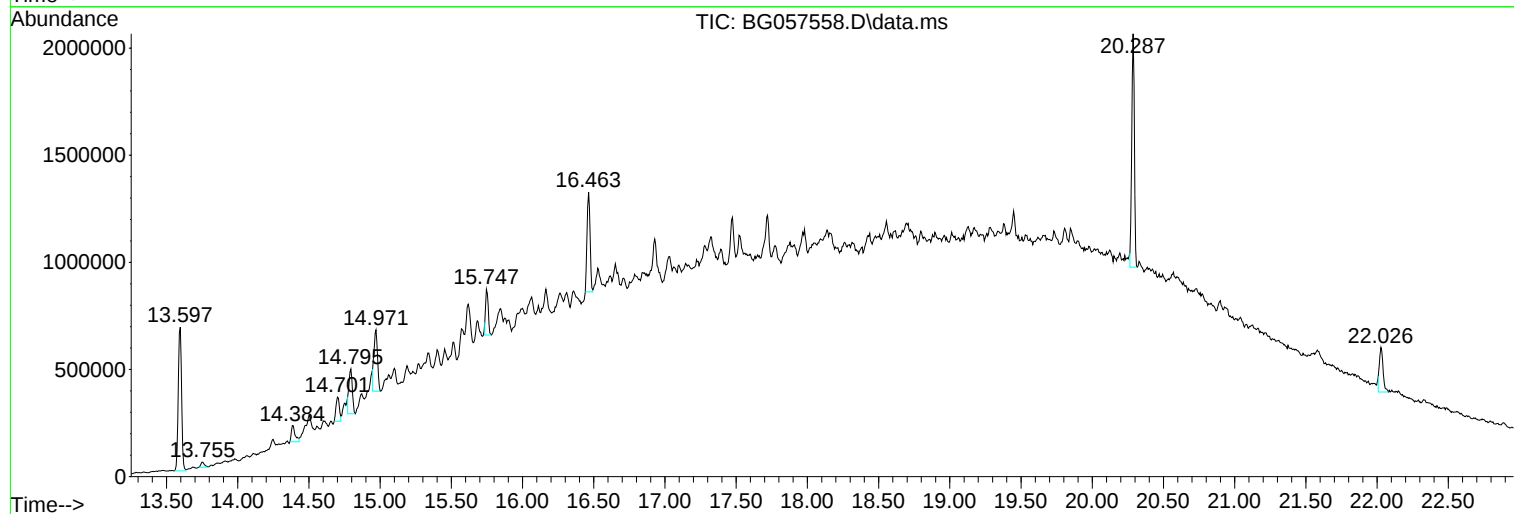
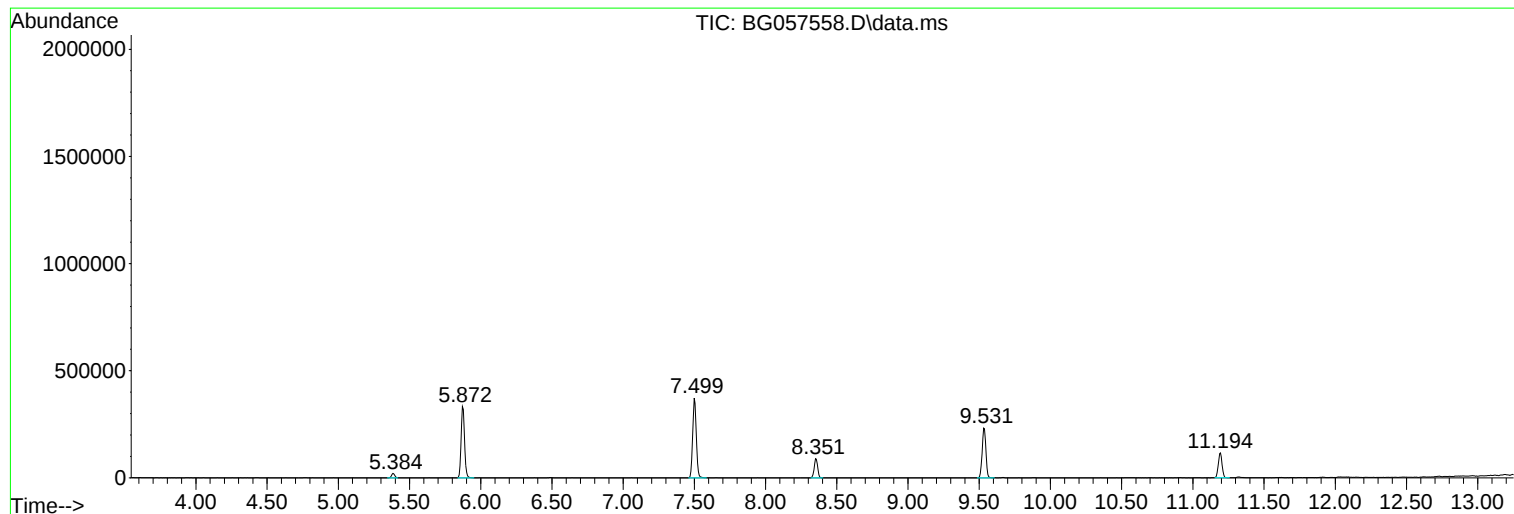
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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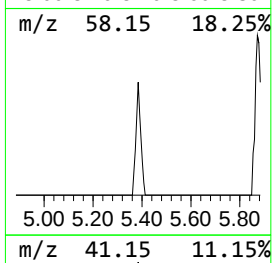
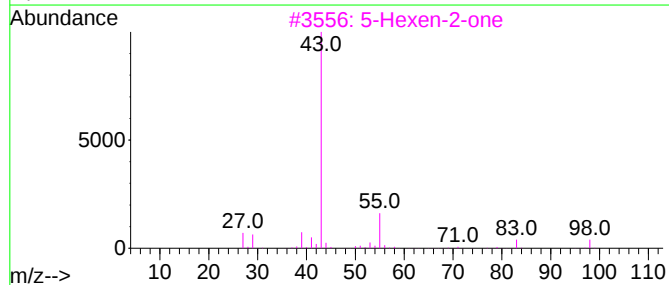
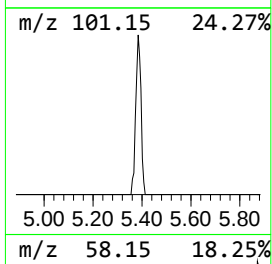
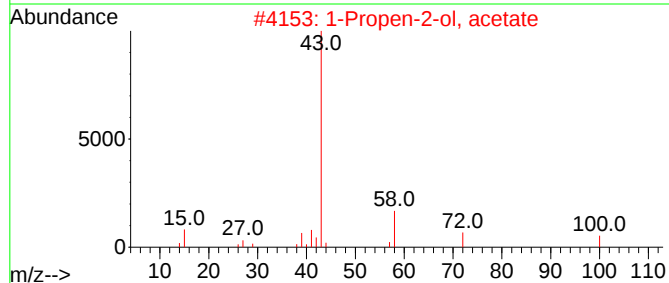
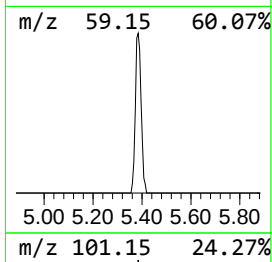
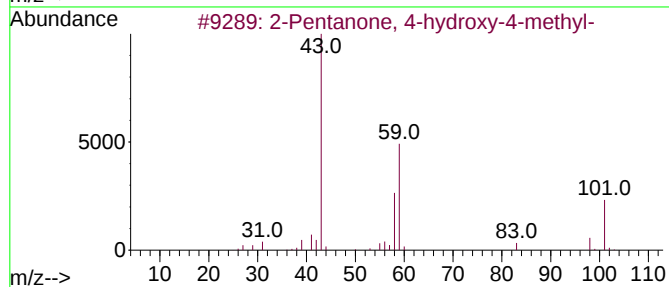
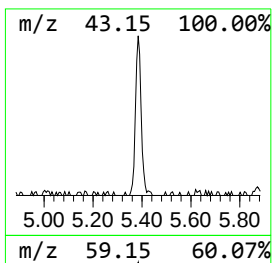
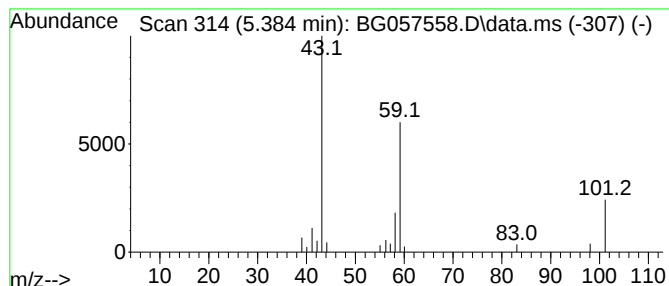
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.384	4.38 ng	32973	1,4-Dichlorobenzene-d4	8.357

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	9
5		3-Octanol	130	C8H18O	000589-98-0	9



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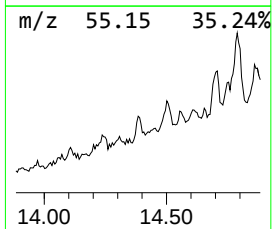
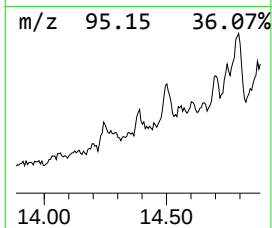
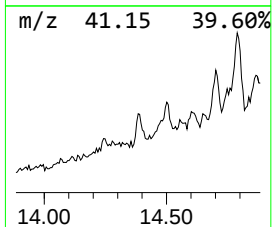
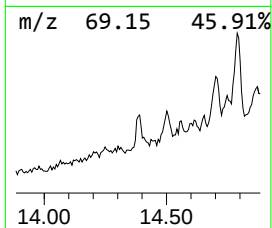
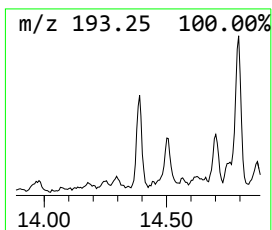
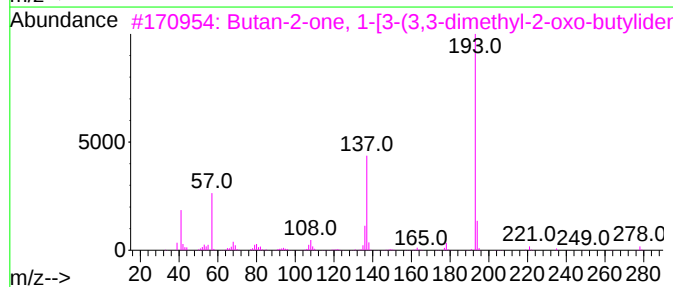
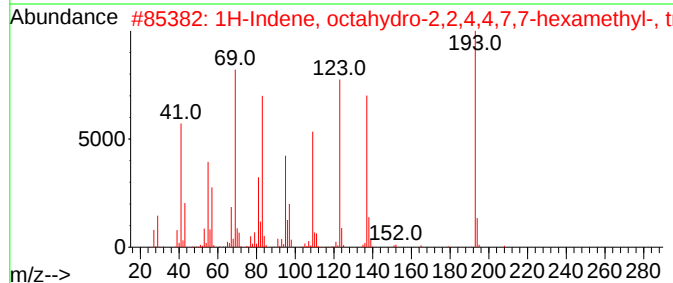
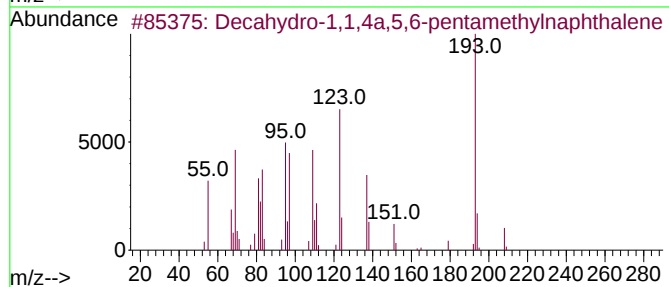
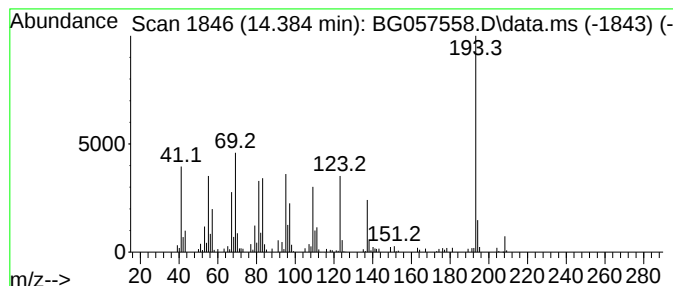
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TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown14.384 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.384	5.86 ng	143578	Acenaphthene-d10	14.977

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	49
2			1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	42
3			Butan-2-one, 1-[3-(3,3-dimethyl-...	278	C16H26N2O2	1000303-34-2	38
4			2-Diethylamino-4-phenylthiooct-2...	302	C18H26N2S	1000090-57-0	37
5			Iminostilbene	193	C14H11N	000256-96-2	35



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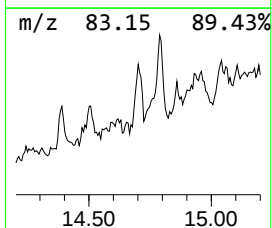
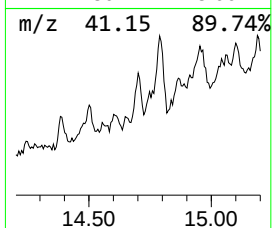
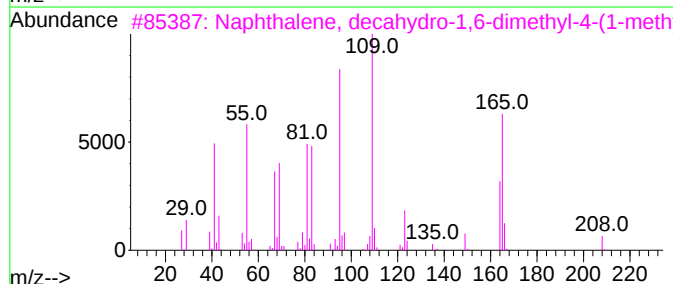
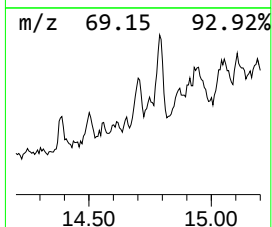
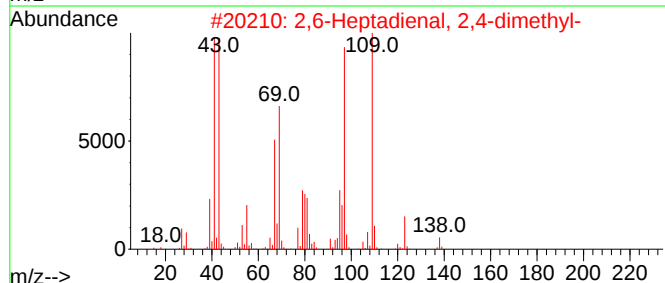
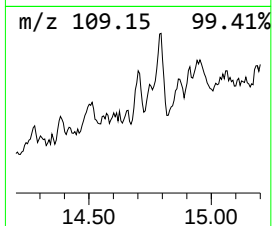
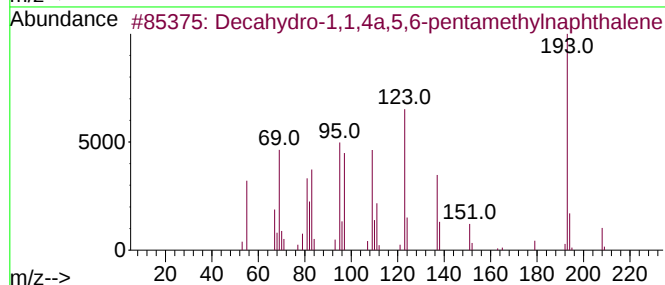
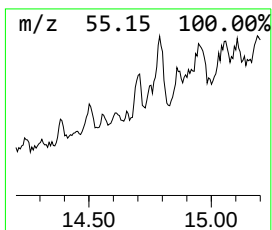
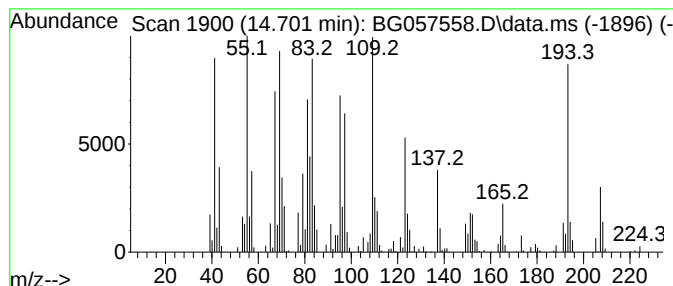
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Peak Number 3 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.701	7.79 ng	190950	Acenaphthene-d10	14.977

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	64
2			2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	45
3			Naphthalene, decahydro-1,6-dimet...	208	C15H28	029788-41-8	43
4			Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	43
5			3-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	040702-26-9	42



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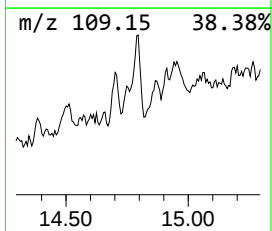
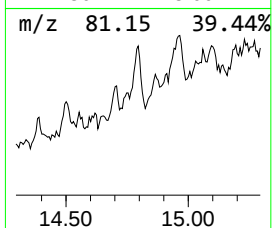
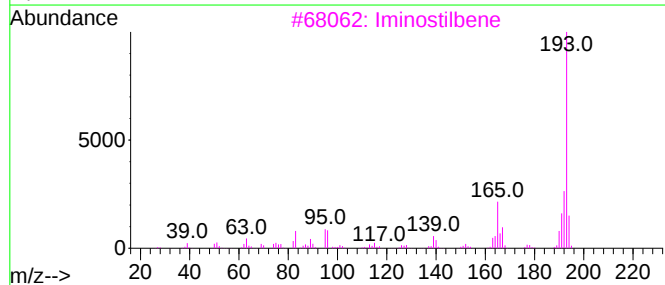
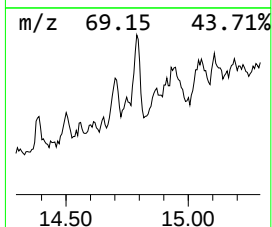
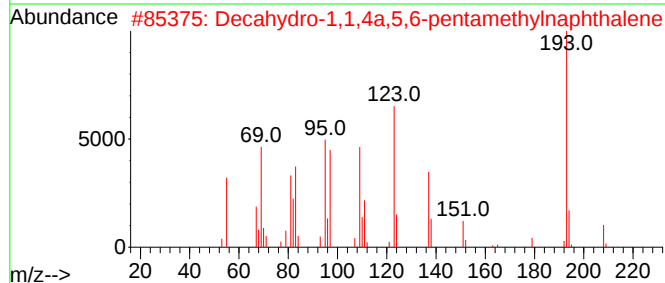
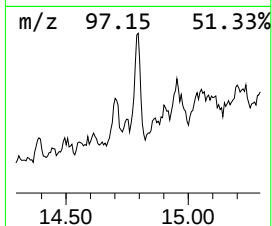
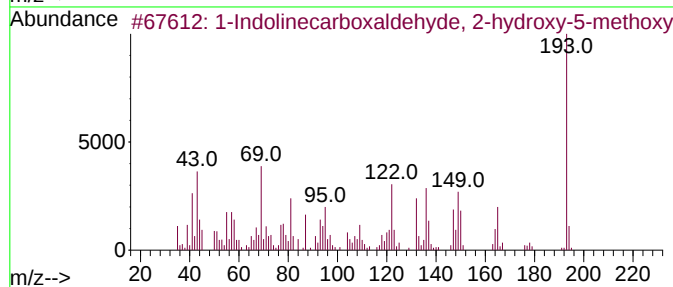
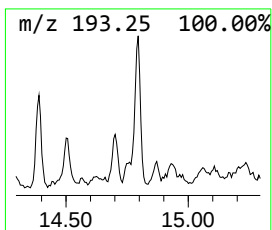
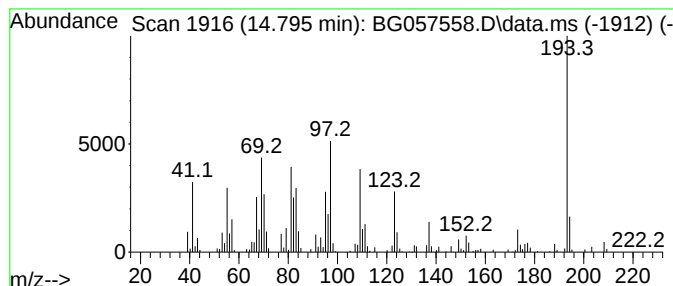
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Peak Number 4 unknown14.795 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.795	14.20 ng	348022	Acenaphthene-d10	14.977

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Indolinecarboxaldehyde, 2-hydr...	193	C10H11NO3	013303-70-3	43		
2	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	43		
3	Iminostilbene	193	C14H11N	000256-96-2	35		
4	S-Phenyl 5-(phenylthio)pentaneth...	302	C17H18OS2	1000234-40-7	32		
5	2-Phenylindolizine	193	C14H11N	025379-20-8	27		



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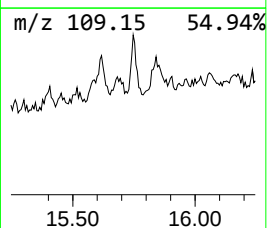
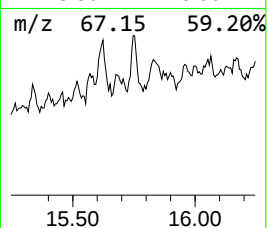
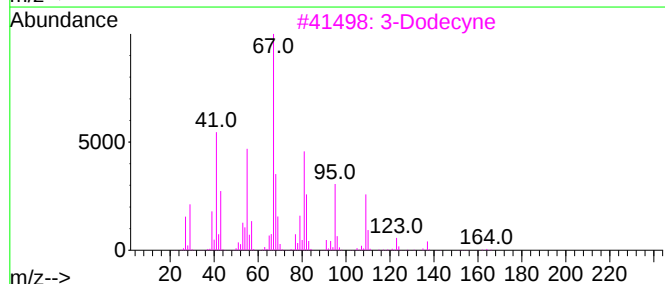
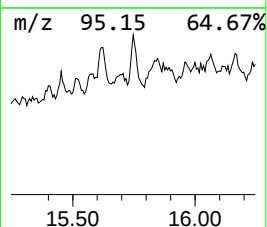
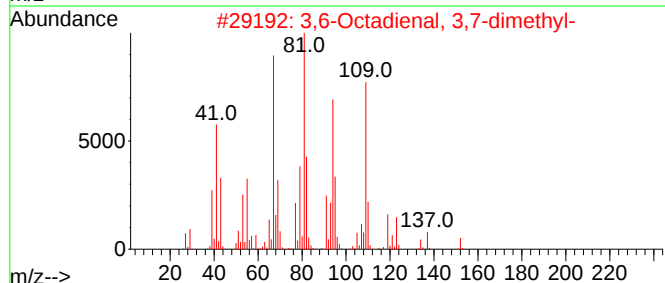
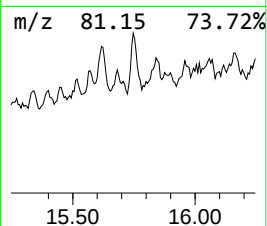
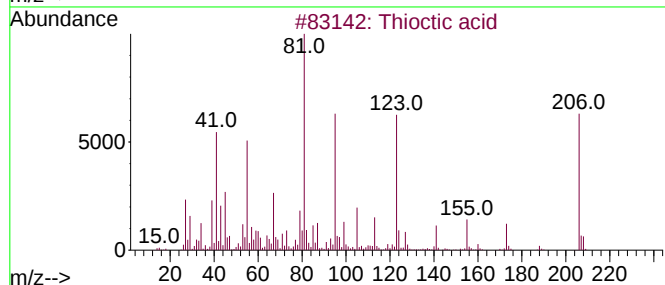
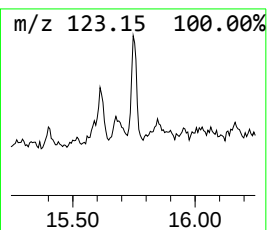
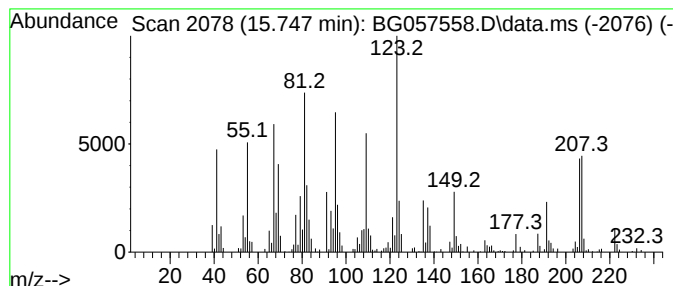
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Peak Number 5 unknown15.747 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.747	10.84 ng	265691	Acenaphthene-d10	14.977

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thioctic acid	206	C8H14O2S2	001077-28-7	43
2			3,6-Octadienal, 3,7-dimethyl-	152	C10H16O	055722-59-3	38
3			3-Dodecyne	166	C12H22	006790-27-8	38
4			cis-3-Methyl-endo-tricyclo[5.2.1...	150	C11H18	1000215-29-0	25
5			Bicyclo[2.2.2]octane, 2-methyl-	124	C9H16	000766-53-0	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.384	4.4	ng	32973	1	8.357	150543	20.0
unknown14.384	14.384	5.9	ng	143578	3	14.977	490086	20.0
Decahydro-1,1,4...	14.701	7.8	ng	190950	3	14.977	490086	20.0
unknown14.795	14.795	14.2	ng	348022	3	14.977	490086	20.0
unknown15.747	15.747	10.8	ng	265691	3	14.977	490086	20.0