

Data Path : Z:\HPCHEM1\BNA G\DATA\BG040918\
 Data File : BG033695.D
 Acq On : 10 Apr 2018 1:25
 Operator : SJ/JU
 Sample : J2282-02
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 EPE-L-6(25-27)

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:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.476	23	32	43	rBV2	65583	150552	4.14%	0.822%
2	3.570	43	48	55	rVB	49457	80890	2.23%	0.442%
3	5.767	416	422	436	rVB2	39097	72686	2.00%	0.397%
4	6.284	503	510	527	rBV	715213	1403301	38.61%	7.666%
5	7.971	789	797	820	rBV	729330	1628134	44.80%	8.894%
6	8.370	857	865	884	rBV	691753	1446638	39.81%	7.903%
7	8.858	941	948	959	rBV	94810	213948	5.89%	1.169%
8	9.193	997	1005	1023	rBV	525443	1057224	29.09%	5.775%
9	10.056	1145	1152	1166	rBV	388769	883336	24.31%	4.825%
10	11.737	1430	1438	1455	rBV	144238	320380	8.82%	1.750%
11	14.105	1828	1841	1861	rBV	1231621	2089609	57.50%	11.415%
12	14.892	1968	1975	1988	rBV	114433	185546	5.11%	1.014%
13	15.474	2067	2074	2085	rBV2	286653	488436	13.44%	2.668%
14	16.038	2165	2170	2176	rVB2	41634	63502	1.75%	0.347%
15	16.237	2199	2204	2209	rVB	34049	43297	1.19%	0.237%
16	16.948	2317	2325	2338	rBV	1203697	1976731	54.39%	10.798%
17	17.089	2346	2349	2358	rVB2	32034	54654	1.50%	0.299%
18	18.206	2530	2539	2555	rBV	407534	715048	19.68%	3.906%
19	19.005	2671	2675	2684	rBV3	42506	71720	1.97%	0.392%
20	20.726	2961	2968	2983	rBV	2621182	3634109	100.00%	19.852%
21	22.066	3191	3196	3208	rVB4	31187	69398	1.91%	0.379%
22	22.548	3271	3278	3290	rBV2	435006	833748	22.94%	4.554%
23	26.302	3903	3917	3936	rBV2	240283	823168	22.65%	4.497%

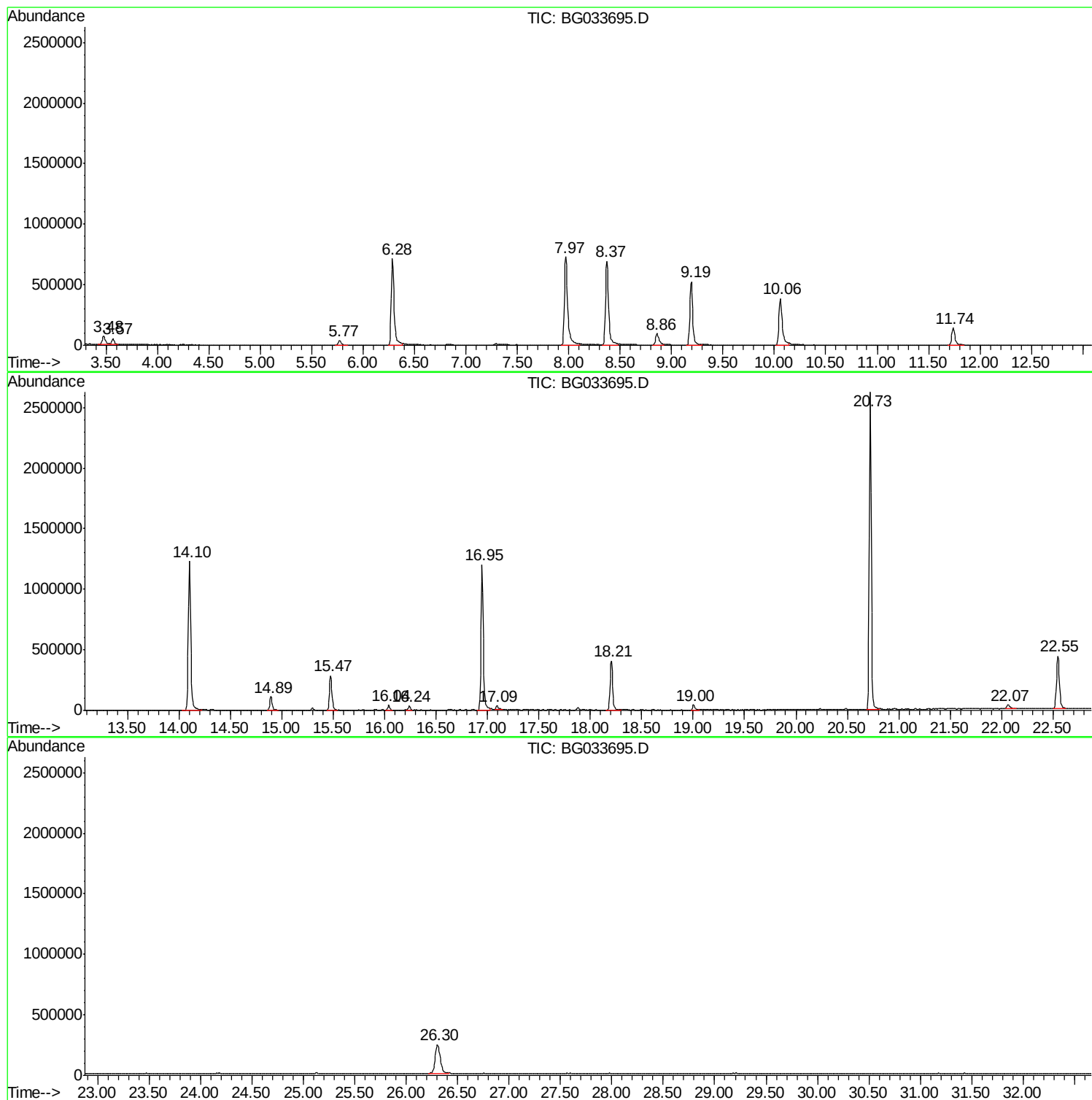
Sum of corrected areas: 18306055

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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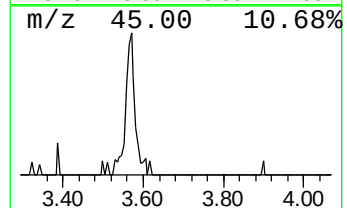
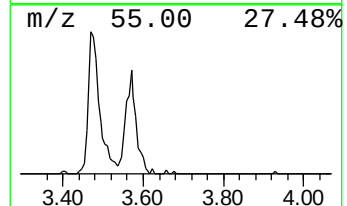
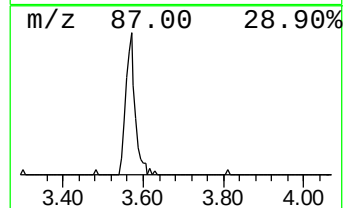
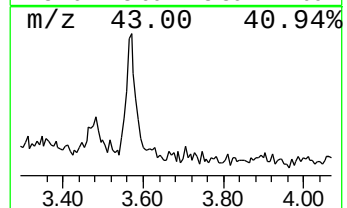
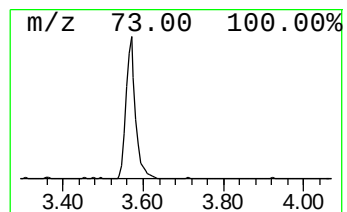
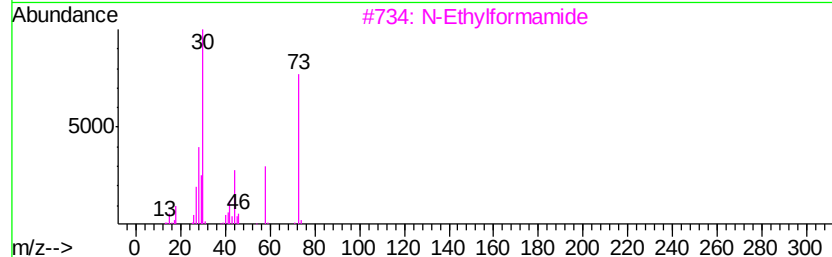
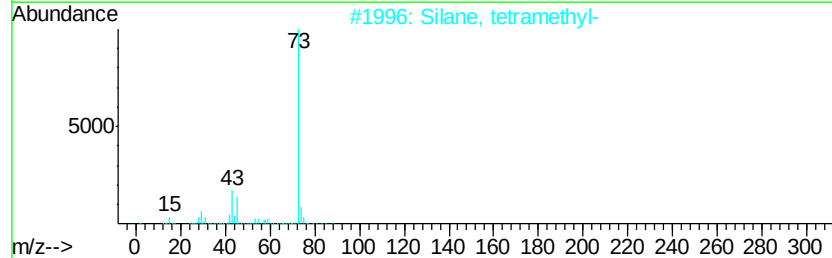
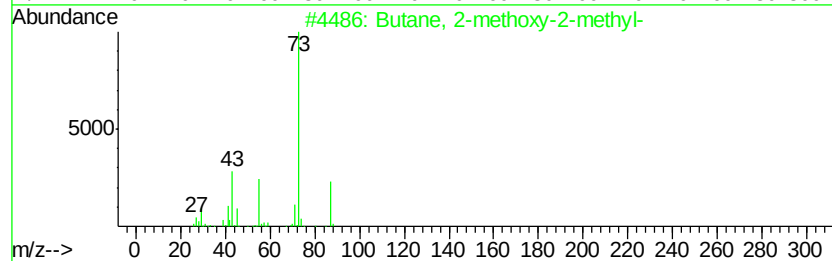
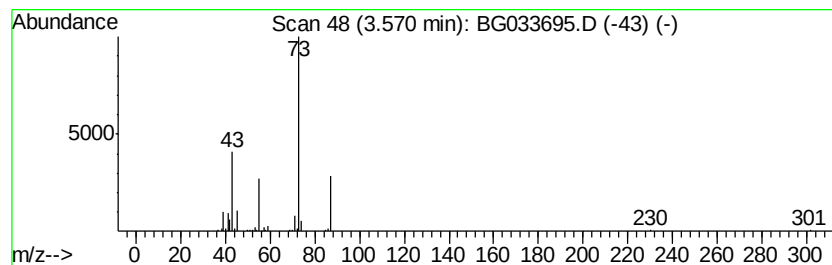
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.57	7.56 ng	80890	1,4-Dichlorobenzene-d4	8.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	47
2		Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		1-Propene-1-thiol	74	C3H6S	000925-89-3	9
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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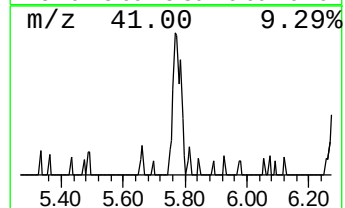
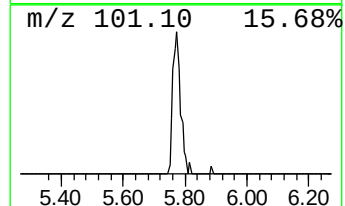
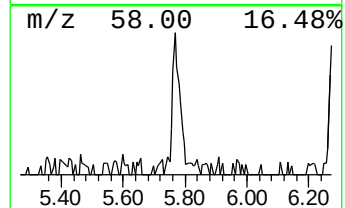
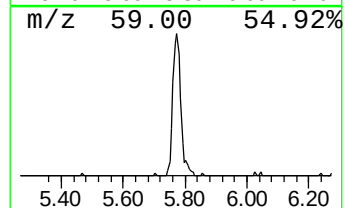
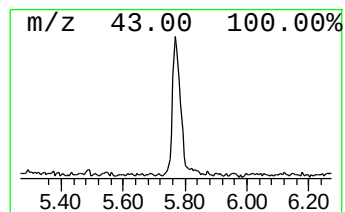
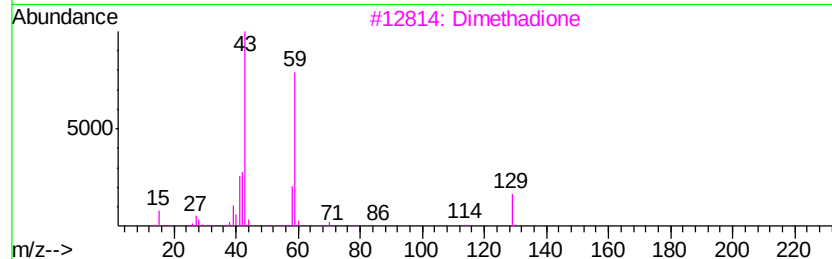
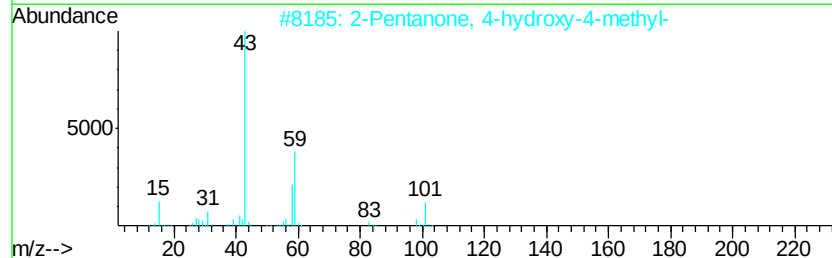
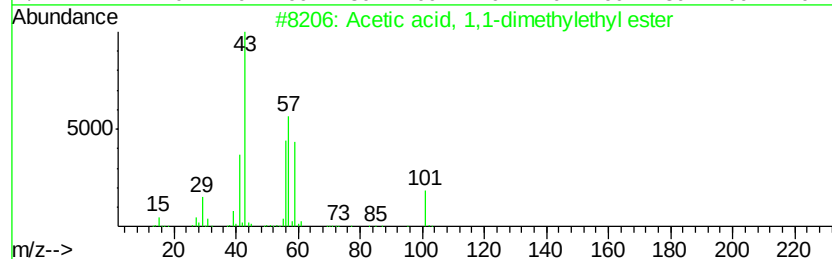
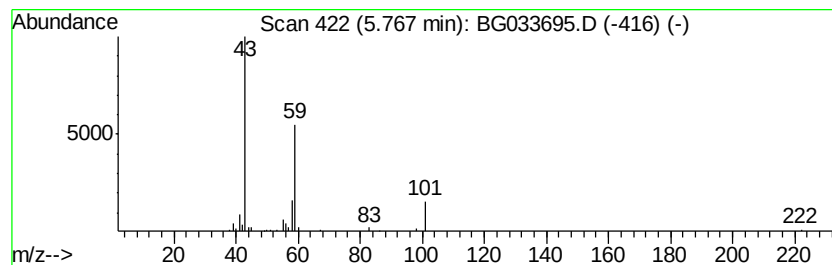
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Peak Number 3 Acetic acid, 1,1-dimethylet... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.77	6.79 ng	72686	1,4-Dichlorobenzene-d4	8.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3		Dimethadione	129	C5H7N03	000695-53-4	42
4		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
5		3-Hexanol	102	C6H14O	000623-37-0	28



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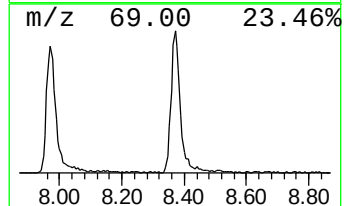
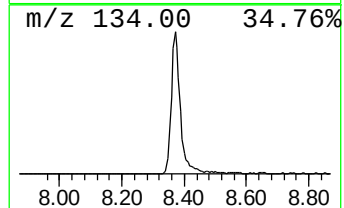
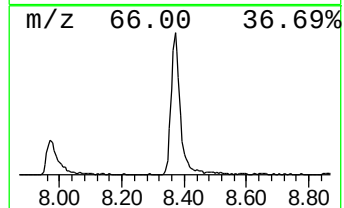
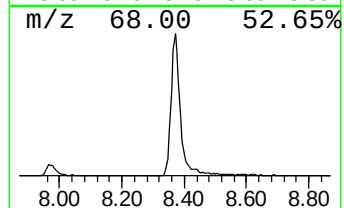
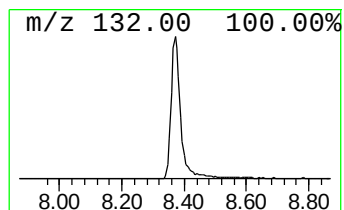
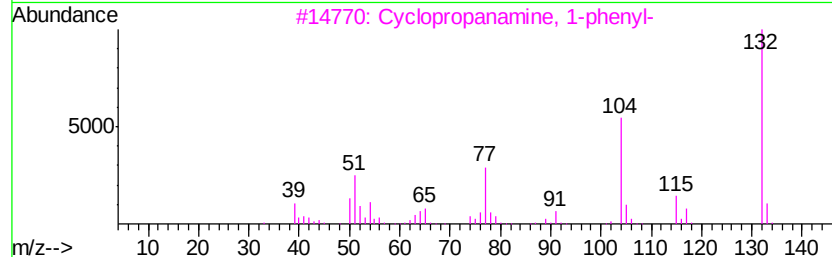
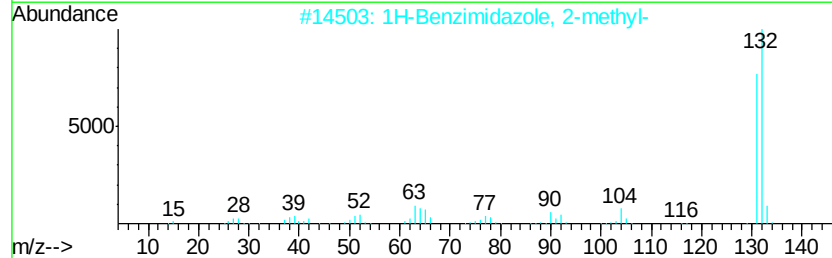
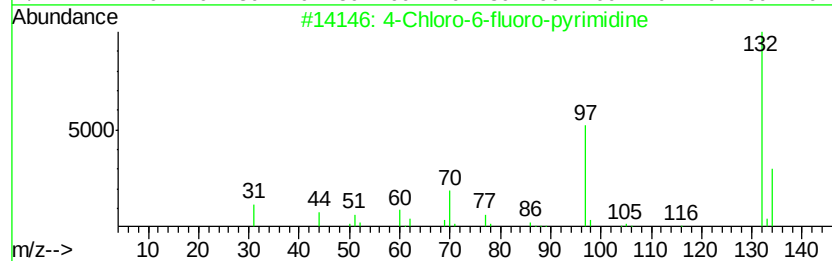
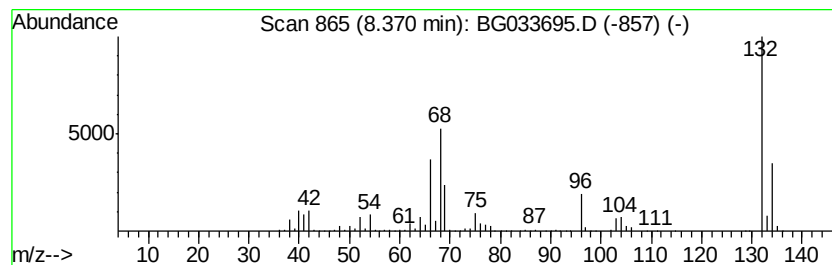
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Peak Number 4 unknown8.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.37	135.23 ng	1446640	1,4-Dichlorobenzene-d4	8.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	22
4		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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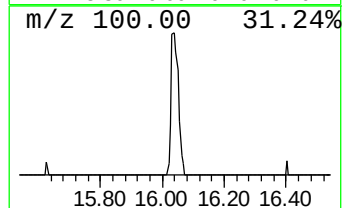
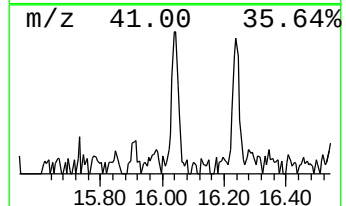
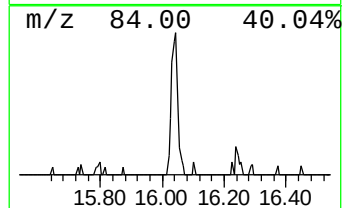
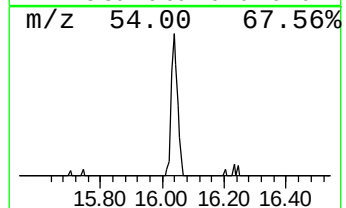
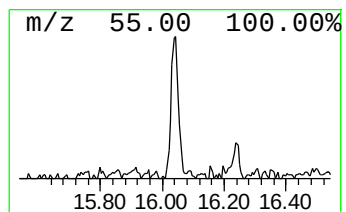
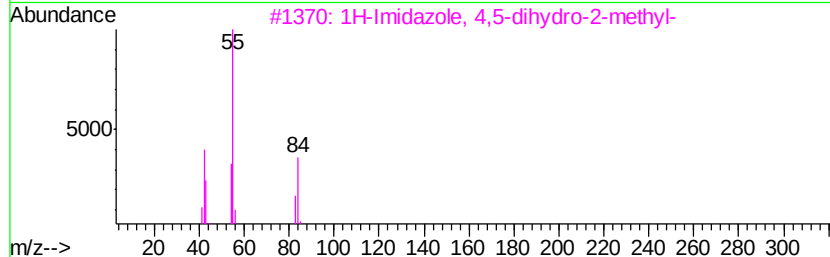
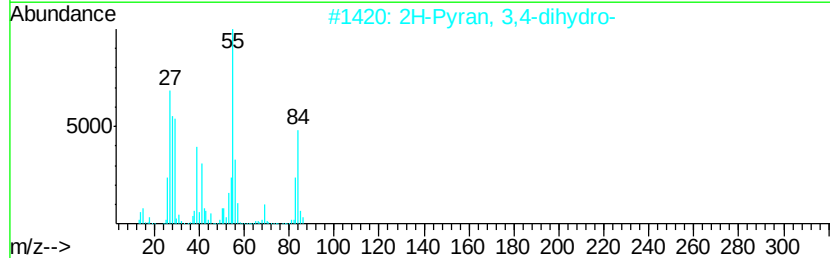
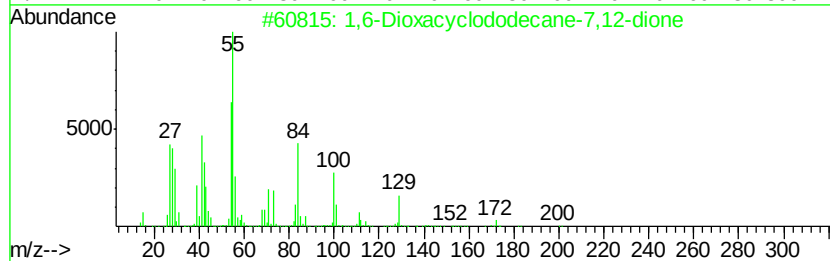
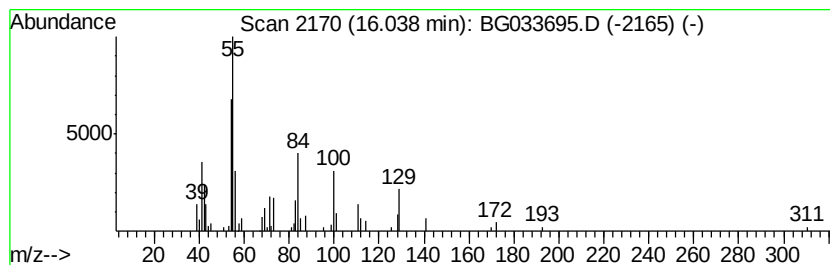
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Peak Number 6 1,6-Dioxacyclododecane-7,12... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.04	2.60 ng	63502	Acenaphthene-d10	15.47

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,6-Dioxacyclododecane-7,12-dione	200	C10H16O4	000777-95-7	80
2			2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	35
3			1H-Imidazole, 4,5-dihydro-2-methyl-	84	C4H8N2	000534-26-9	25
4			Hydracrylic acid, monoanhydride ...	156	C7H13BO3	033823-94-8	25
5			Oxacycloundecane-2,7-dione	184	C10H16O3	004753-58-6	23



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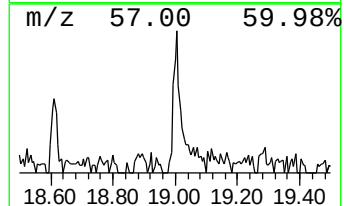
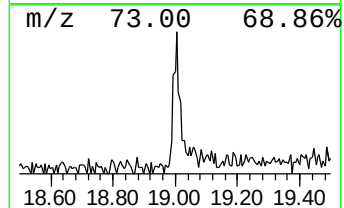
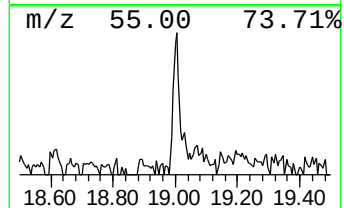
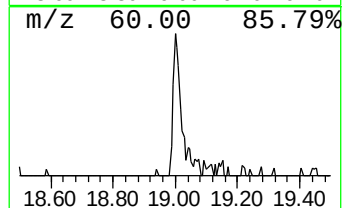
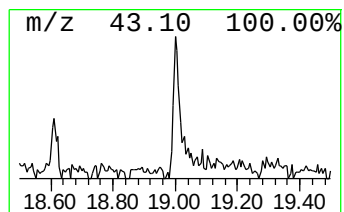
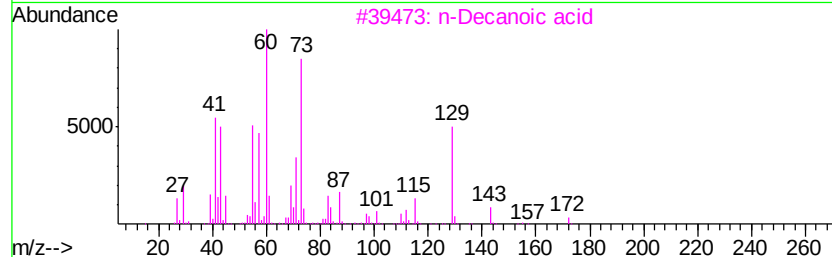
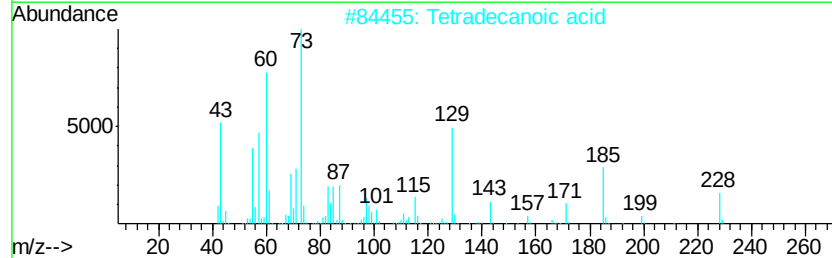
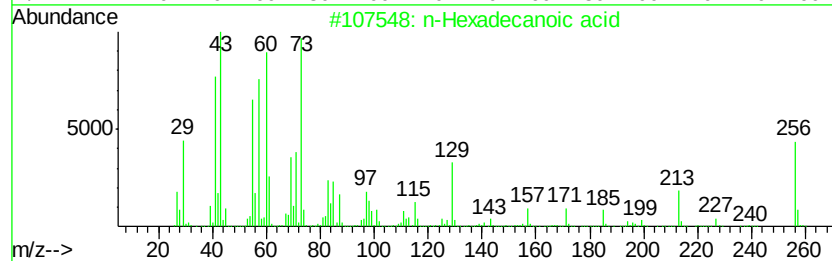
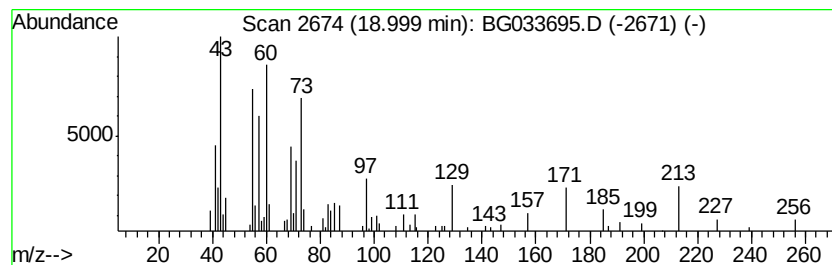
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Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
19.00	2.01 ng	71720	Phenanthrene-d10		18.21
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
3	n-Decanoic acid	172	C10H20O2	000334-48-5	52
4	Tridecanoic acid	214	C13H26O2	000638-53-9	50
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	43



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TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.57	7.6	ng	80890	1	8.86	213948	20.0
Acetic acid, 1,1-...	5.77	6.8	ng	72686	1	8.86	213948	20.0
unknown8.37	8.37	135.2	ng	1446640	1	8.86	213948	20.0
1,6-Dioxacyclodod...	16.04	2.6	ng	63502	3	15.47	488436	20.0
n-Hexadecanoic acid	19.00	2.0	ng	71720	4	18.21	715048	20.0