

Data Path : Z:\HPCHEM1\BNA G\DATA\BG040318\
 Data File : BG033550.D
 Acq On : 4 Apr 2018 8:14
 Operator : SJ/JU
 Sample : J2177-07
 Misc :
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 032818-JETB-F-D-B

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	3.483	27	33	42	rBV	141117	279289	7.08%	1.850%
2	3.571	43	48	61	rVB	112782	195992	4.97%	1.299%
3	5.774	417	423	432	rVB2	26564	47881	1.21%	0.317%
4	6.297	506	512	533	rBV	138869	332313	8.43%	2.202%
5	7.983	793	799	829	rBV2	87770	276344	7.01%	1.831%
6	8.377	860	866	881	rBV	314565	698750	17.72%	4.630%
7	8.865	943	949	959	rBV2	77763	183421	4.65%	1.215%
8	9.199	996	1006	1020	rBV	472140	966477	24.51%	6.403%
9	10.063	1146	1153	1179	rBV	376395	916115	23.23%	6.070%
10	11.749	1432	1440	1451	rBV	135860	301051	7.63%	1.995%
11	14.105	1834	1841	1859	rBV	1311916	2355461	59.73%	15.606%
12	14.899	1966	1976	1985	rBV2	25215	45782	1.16%	0.303%
13	15.480	2069	2075	2084	rBV2	304682	538726	13.66%	3.569%
14	16.955	2318	2326	2339	rBV	815927	1432386	36.32%	9.490%
15	18.212	2533	2540	2554	rBV2	454868	792638	20.10%	5.252%
16	20.733	2963	2969	2985	rBV	2906380	3943484	100.00%	26.128%
17	22.073	3193	3197	3206	rBV4	54658	105193	2.67%	0.697%
18	22.560	3272	3280	3294	rBV	429951	887499	22.51%	5.880%
19	26.326	3910	3921	3938	rBV	223510	794262	20.14%	5.262%

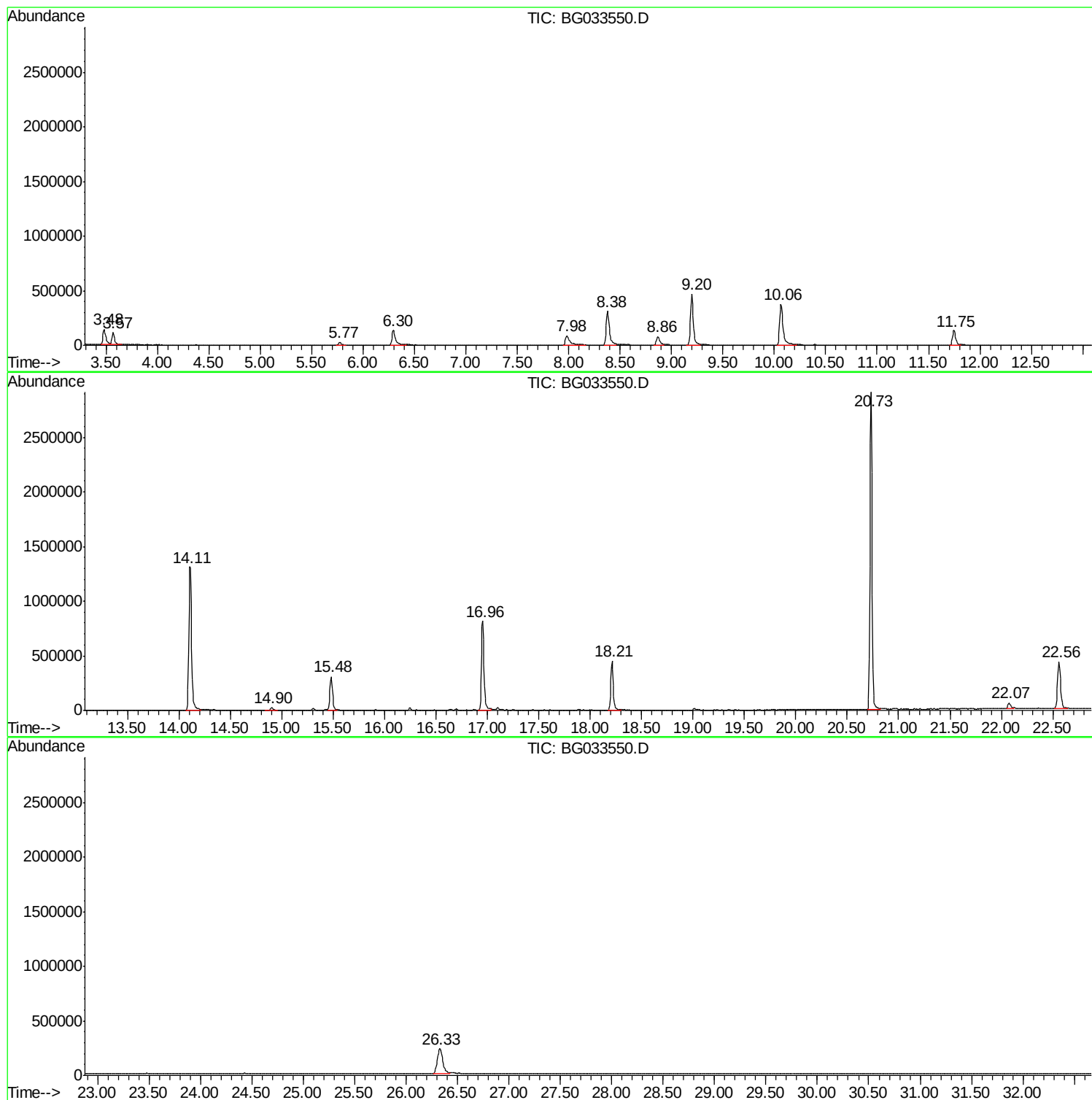
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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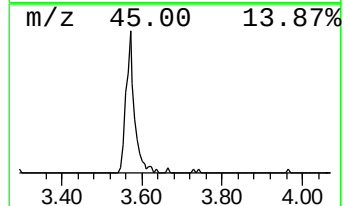
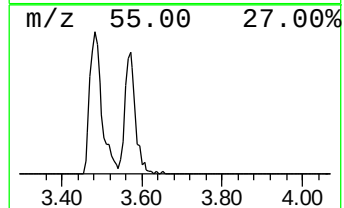
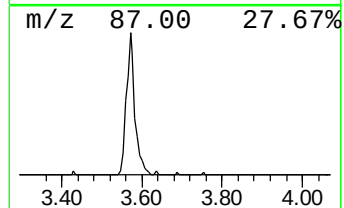
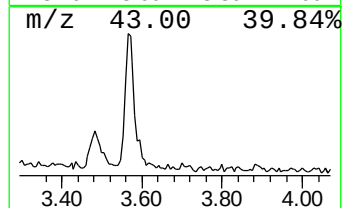
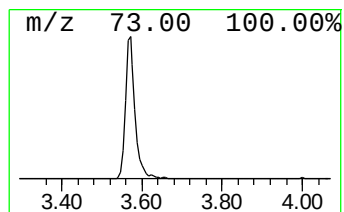
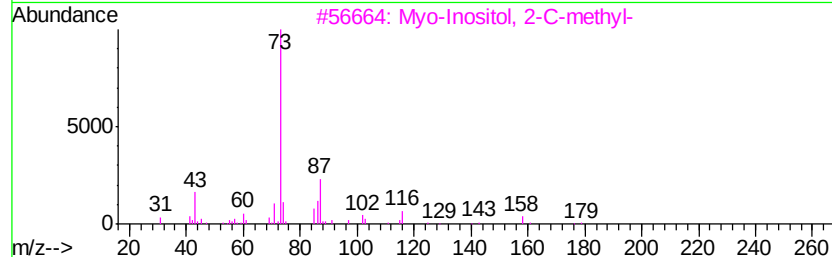
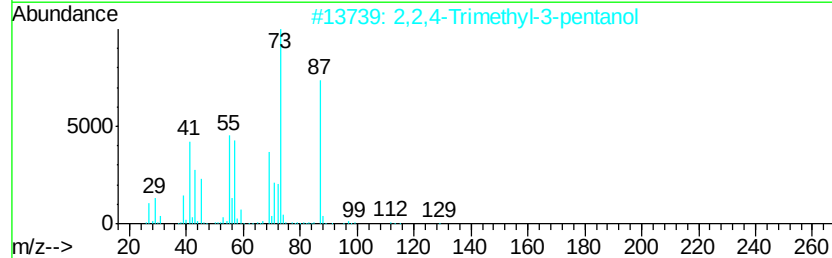
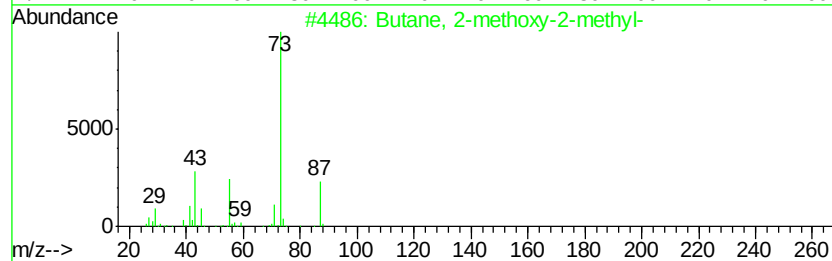
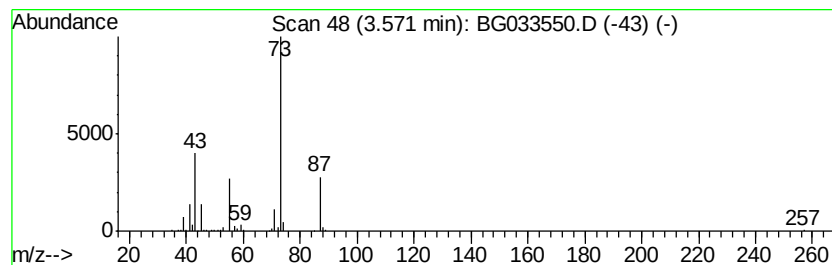
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.57	21.37 ng	195992	1,4-Dichlorobenzene-d4	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Myo-Inositol, 2-C-methyl-	194	C7H14O6	000472-96-8	33
4		Myo-Inositol, 4-C-methyl-	194	C7H14O6	000472-95-7	33
5		Butanoic acid, 2-hydroxy-2-methyl-	132	C6H12O3	032793-34-3	23



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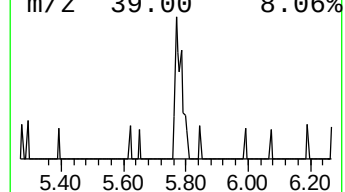
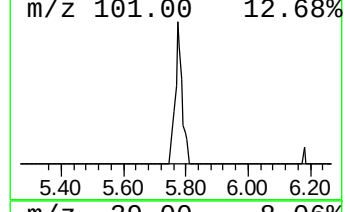
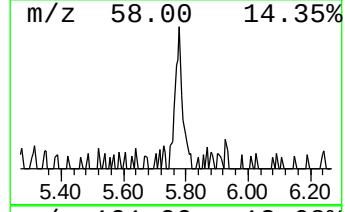
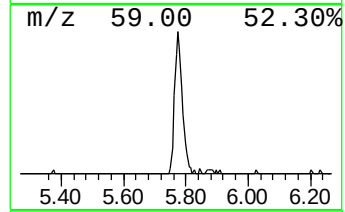
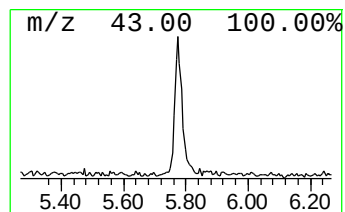
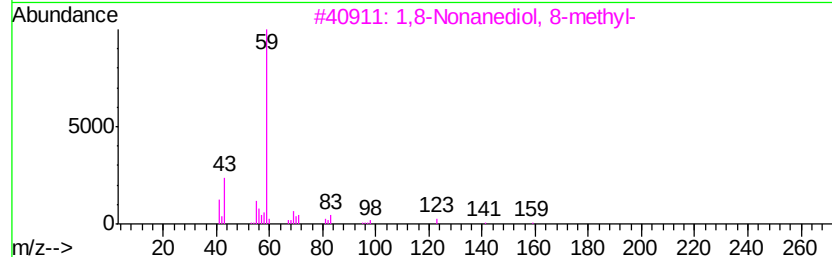
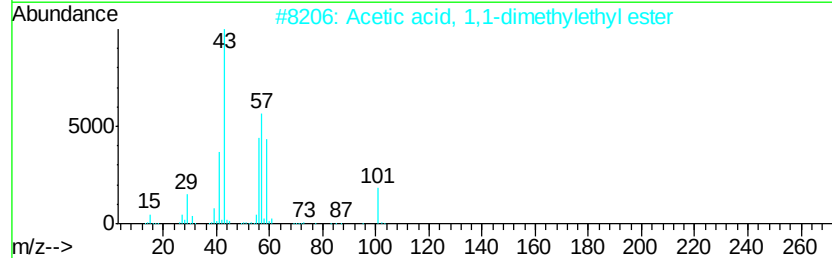
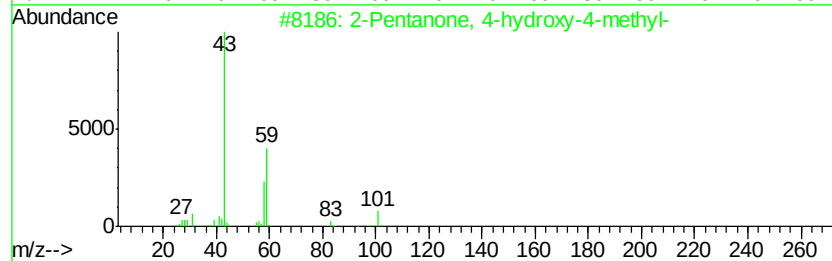
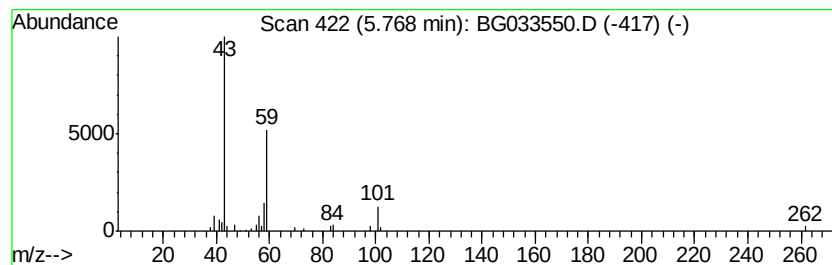
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.77	5.22 ng	47881	1,4-Dichlorobenzene-d4	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	45
3		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	17
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		2-Propanone, 1-cyclopropyl-	98	C6H10O	004160-75-2	9



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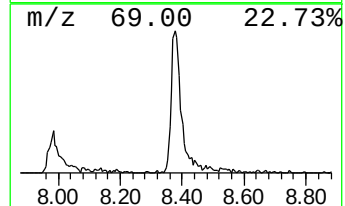
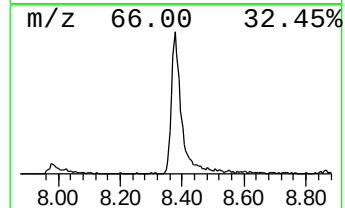
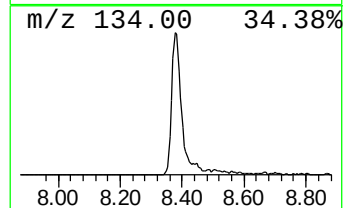
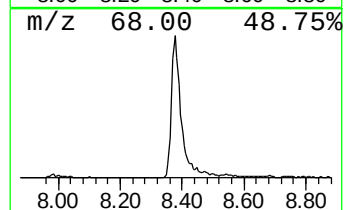
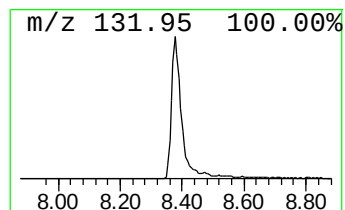
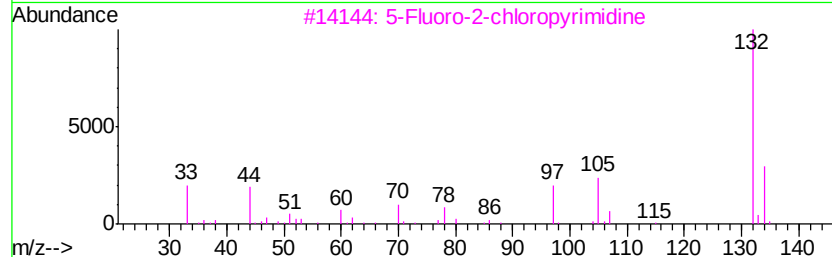
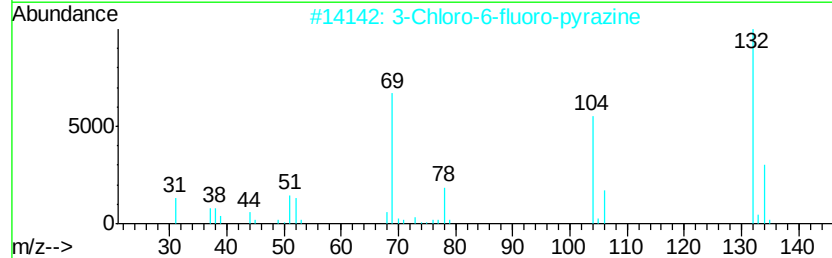
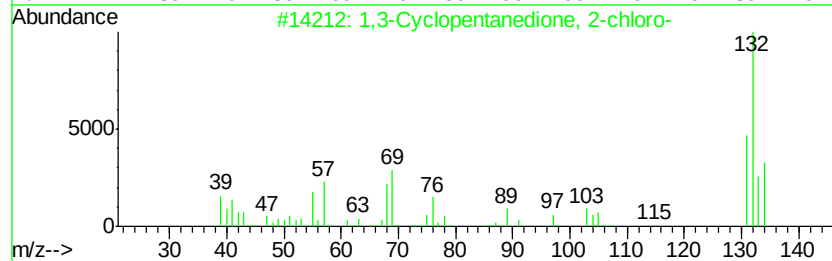
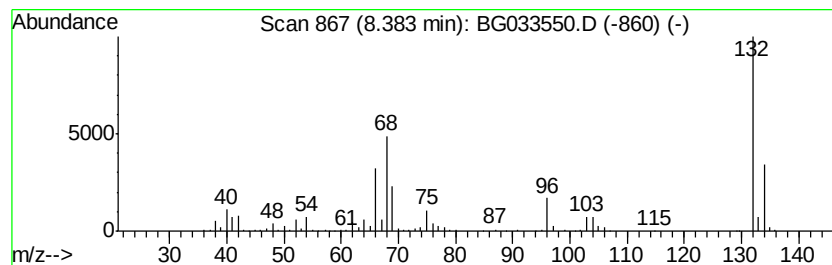
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Peak Number 4 unknown8.38 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.38	76.19 ng	698750	1,4-Dichlorobenzene-d4	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	23
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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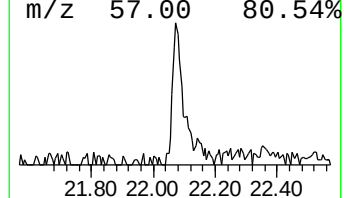
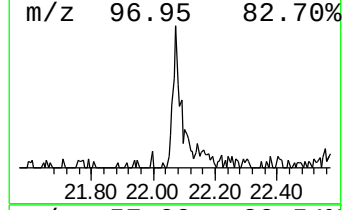
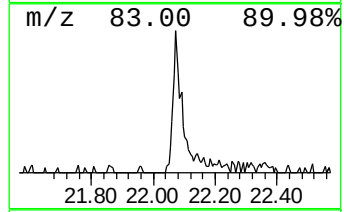
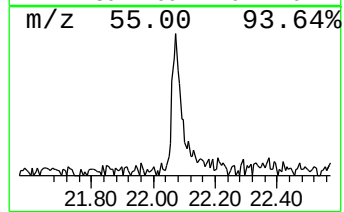
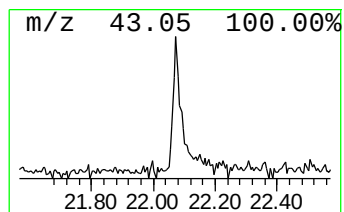
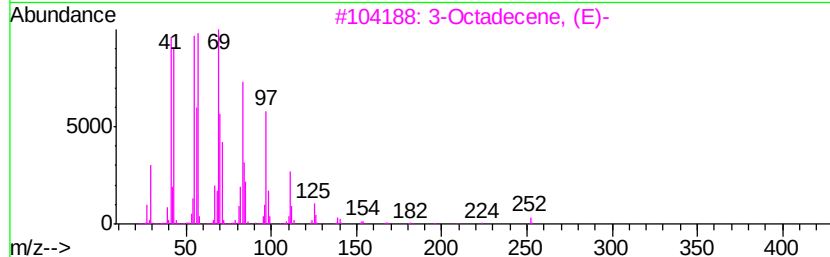
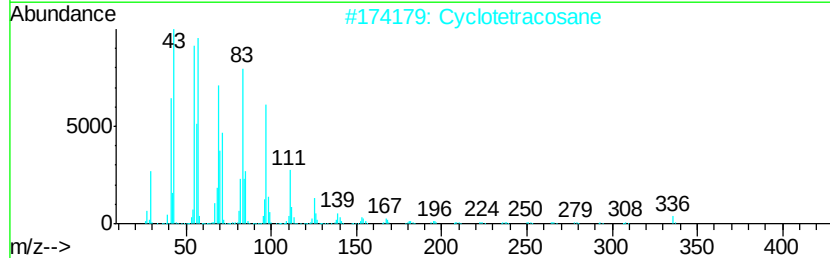
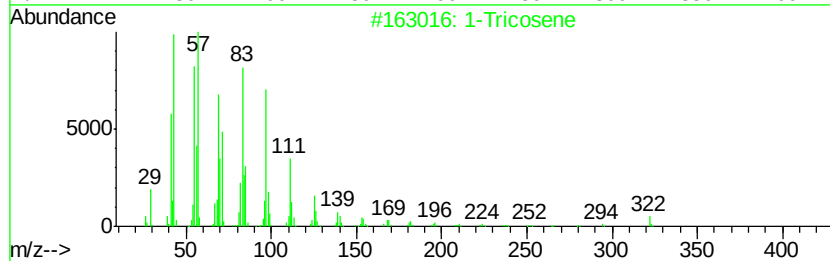
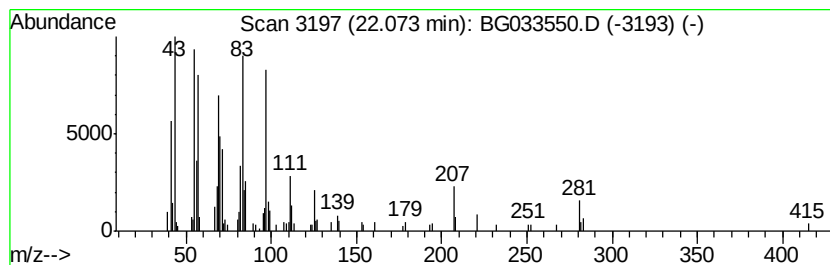
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Peak Number 6 1-Tricosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.07	2.37 ng	105193	Chrysene-d12	22.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Tricosene	322	C23H46	018835-32-0	87
2		Cyclotetracosane	336	C24H48	000297-03-0	83
3		3-Octadecene, (E)-	252	C18H36	007206-19-1	80
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	76
5		1-Octadecene	252	C18H36	000112-88-9	70



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.57	21.4	ng	195992	1	8.87	183421	20.0
2-Pentanone, 4-hy...	5.77	5.2	ng	47881	1	8.87	183421	20.0
unknown8.38	8.38	76.2	ng	698750	1	8.87	183421	20.0
1-Tricosene	22.07	2.4	ng	105193	5	22.56	887499	20.0