

Data Path : Z:\HPCHEM1\BNA G\DATA\BG032818\
 Data File : BG033397.D
 Acq On : 28 Mar 2018 22:06
 Operator : SJ/JU
 Sample : J2097-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 LIP-16

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	3.481	26	33	44	rBV	168091	355399	8.47%	1.911%
2	3.575	44	49	56	rVB	104350	157977	3.76%	0.850%
3	5.779	417	424	430	rBV2	26722	46458	1.11%	0.250%
4	6.301	506	513	531	rBV	303183	590349	14.06%	3.175%
5	7.988	792	800	811	rBV	170385	389432	9.28%	2.094%
6	8.381	859	867	882	rBV	634108	1259831	30.01%	6.775%
7	8.863	941	949	959	rBV	137650	275593	6.56%	1.482%
8	9.198	998	1006	1020	rBV	658938	1261314	30.04%	6.783%
9	10.068	1145	1154	1174	rBV	500824	1115415	26.57%	5.998%
10	11.748	1432	1440	1451	rBV	207986	405647	9.66%	2.181%
11	14.110	1833	1842	1856	rBV	1716400	2844124	67.74%	15.294%
12	14.903	1972	1977	1983	rBV2	41906	60812	1.45%	0.327%
13	15.485	2067	2076	2088	rBV2	390931	647703	15.43%	3.483%
14	16.960	2319	2327	2339	rBV	1253654	2073913	49.40%	11.153%
15	18.211	2533	2540	2553	rBV	457593	805024	19.17%	4.329%
16	19.016	2672	2677	2688	rBV2	59252	123835	2.95%	0.666%
17	20.250	2882	2887	2894	rBV7	30207	63365	1.51%	0.341%
18	20.737	2963	2970	2979	rBV	3086460	4198429	100.00%	22.577%
19	22.071	3193	3197	3206	rBV3	77455	129183	3.08%	0.695%
20	22.559	3273	3280	3292	rBV2	455904	896059	21.34%	4.819%
21	26.331	3911	3922	3934	rBV3	259502	895882	21.34%	4.818%

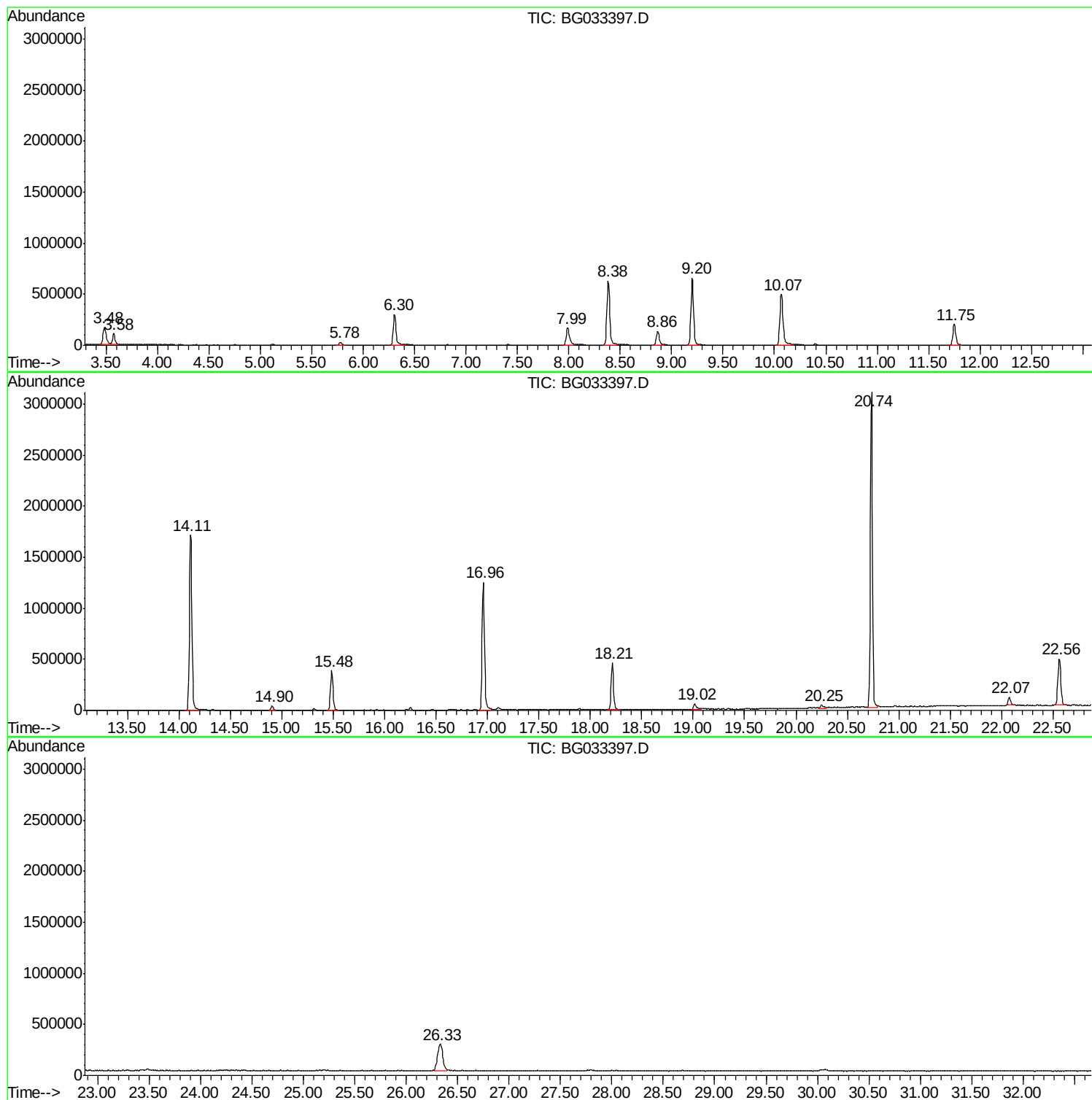
Sum of corrected areas: 18595744

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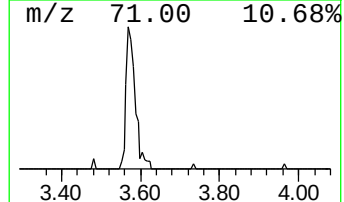
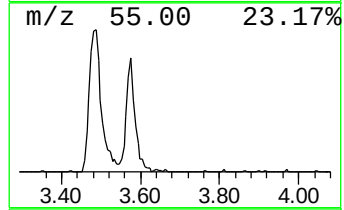
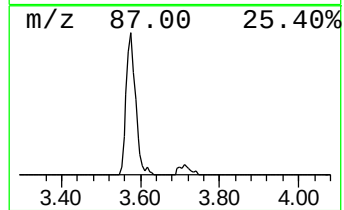
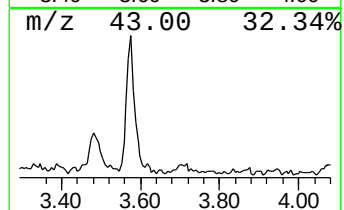
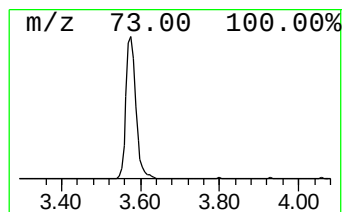
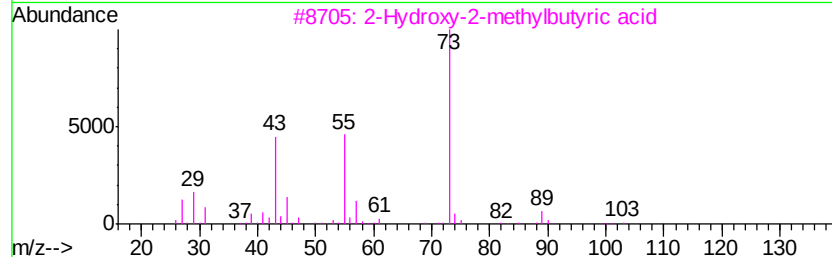
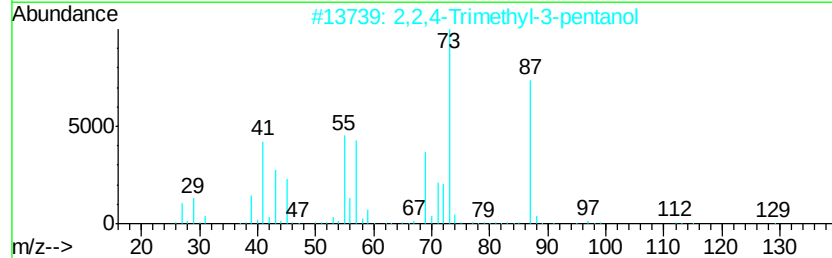
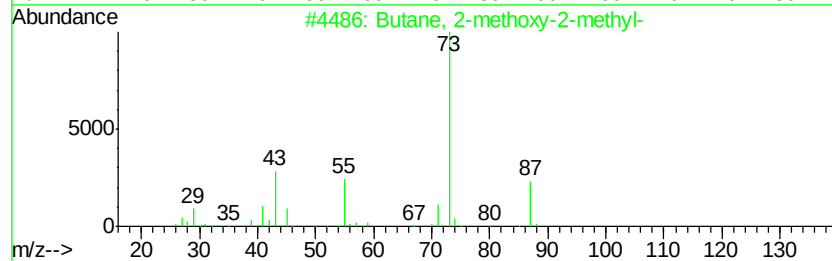
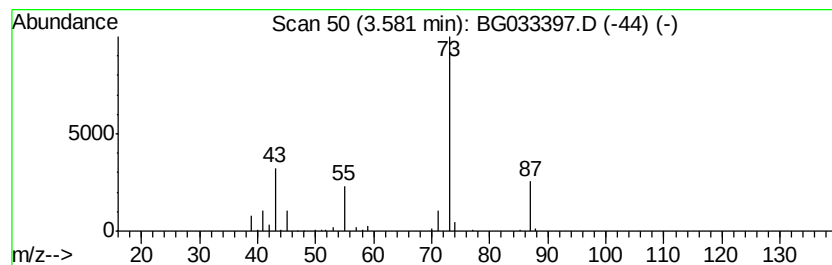
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.58	11.46 ng	157977	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	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	23
4		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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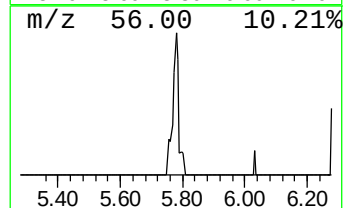
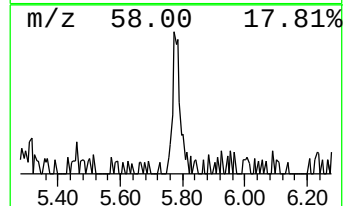
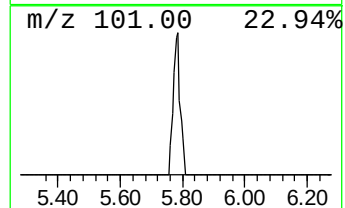
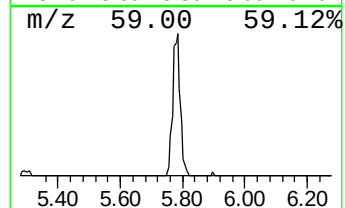
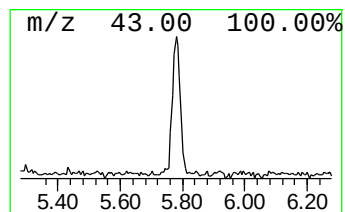
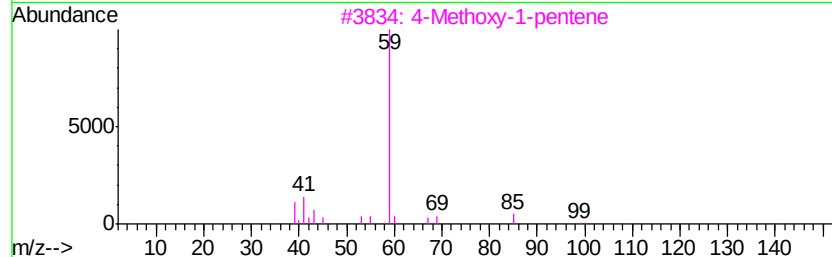
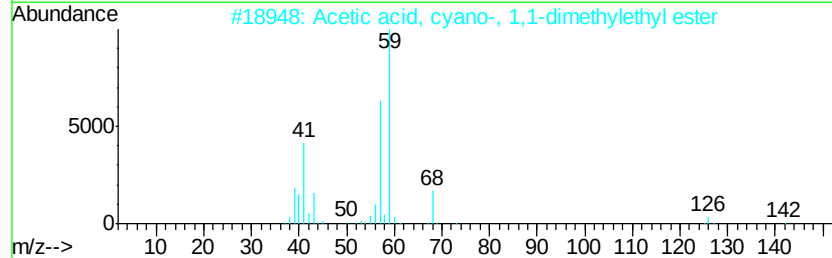
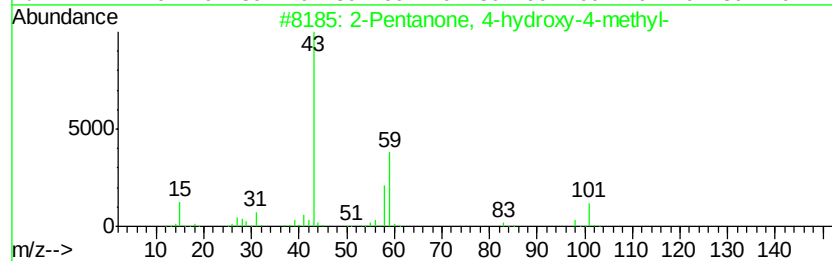
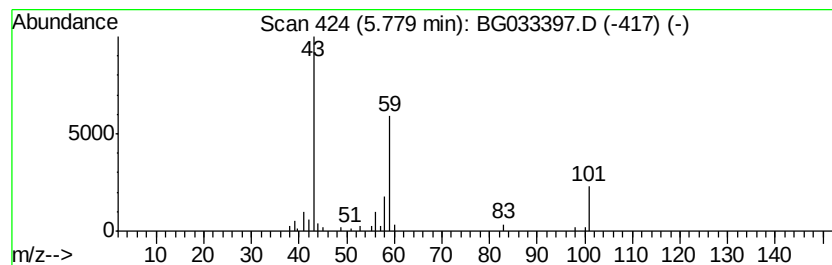
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.78	3.37 ng	46458	1,4-Dichlorobenzene-d4	8.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3	4-Methoxy-1-pentene	100	C6H12O	098386-09-5	12
4	Oxirane, tetramethyl-	100	C6H12O	005076-20-0	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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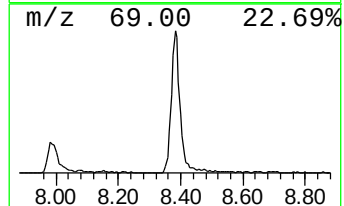
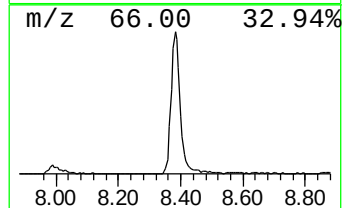
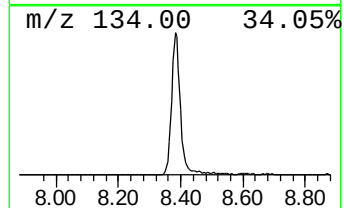
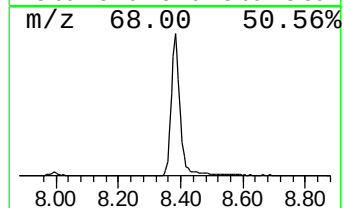
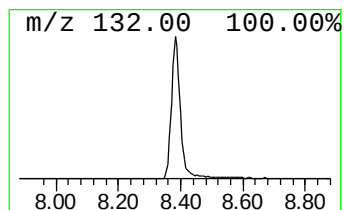
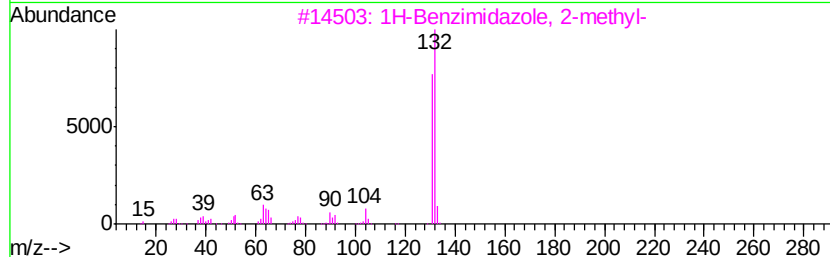
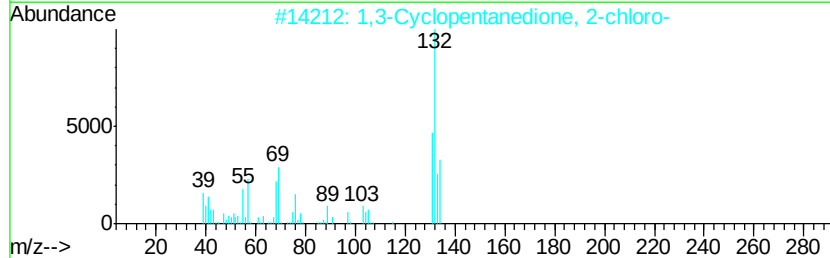
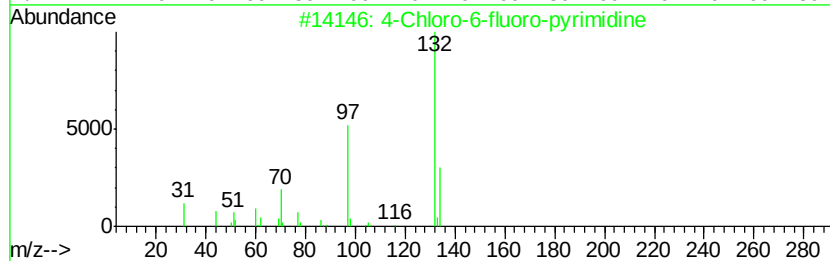
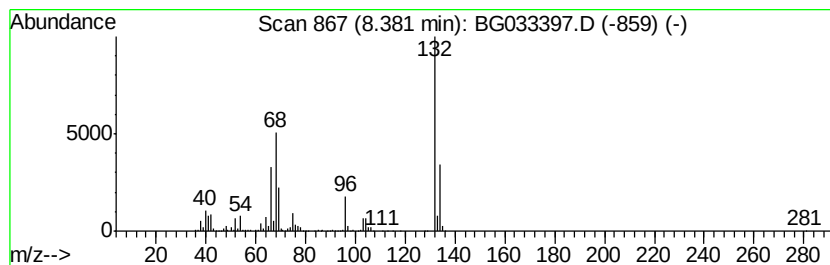
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Peak Number 4 unknown8.38 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.38	91.43 ng	1259830	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		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Aminoindole	132	C8H8N2	005192-03-0	22
5		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16



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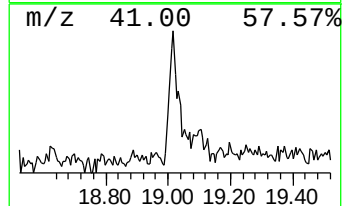
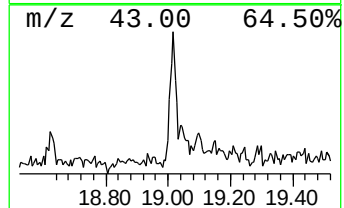
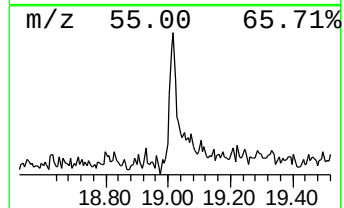
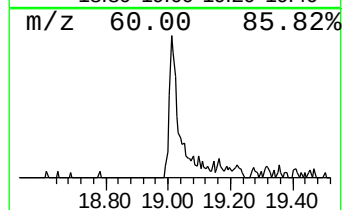
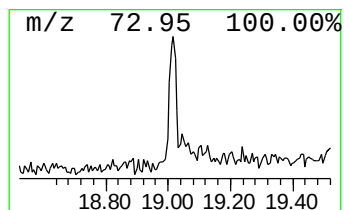
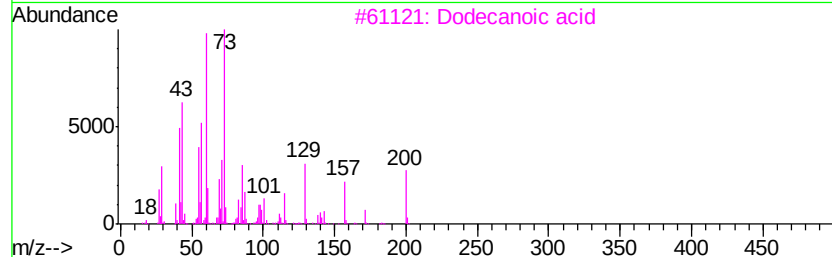
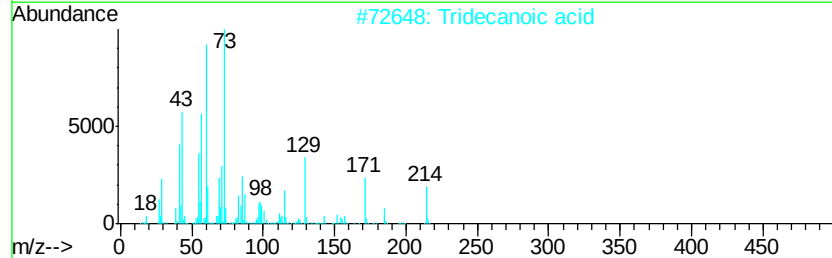
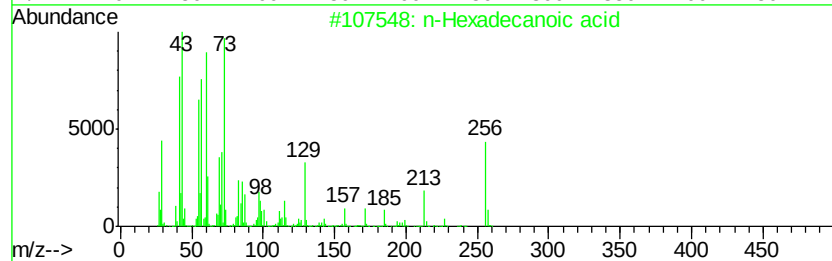
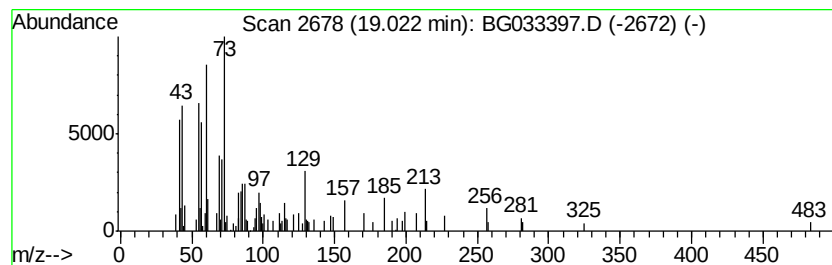
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.02	3.08 ng	123835	Phenanthrene-d10	18.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
2	Tridecanoic acid	214	C13H26O2	000638-53-9	64
3	Dodecanoic acid	200	C12H24O2	000143-07-7	62
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	l-(+)-Ascorbic acid 2,6-dihexade...	652	C38H68O8	028474-90-0	52



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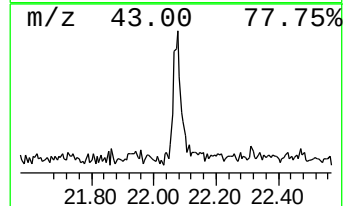
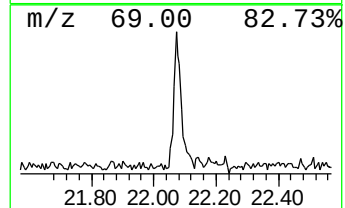
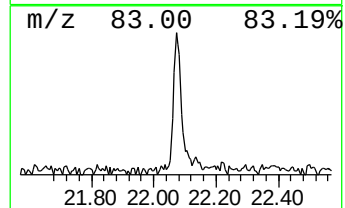
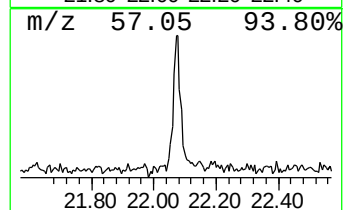
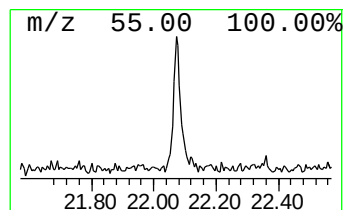
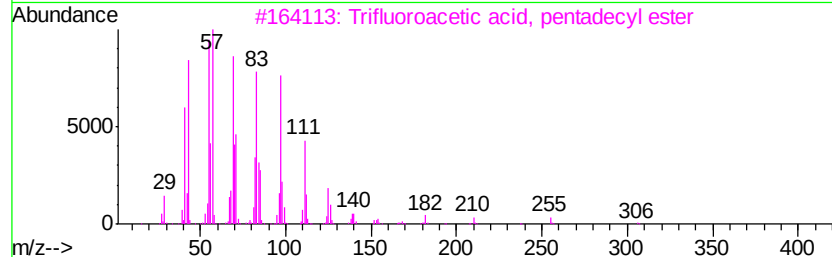
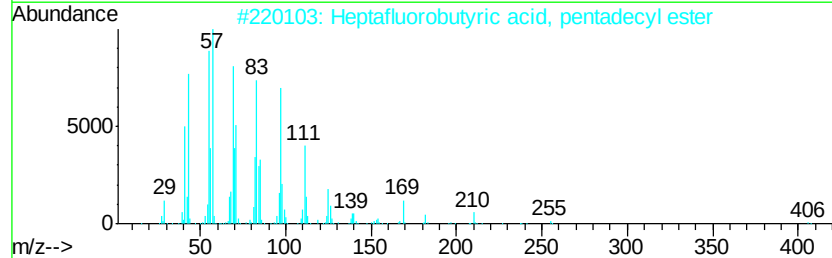
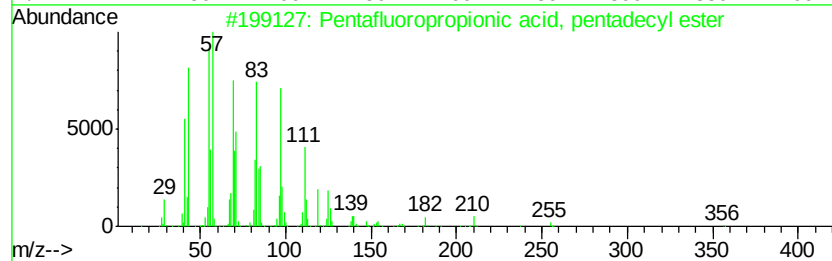
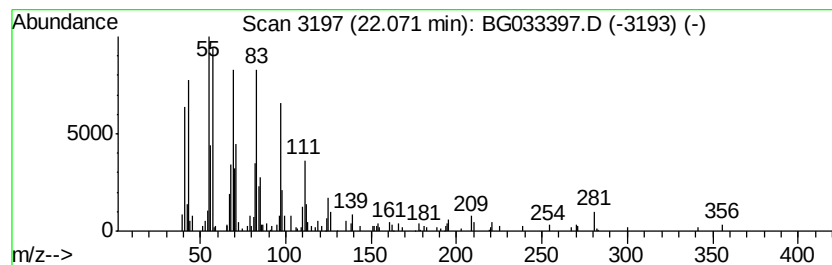
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Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.07	2.88 ng	129183	Chrysene-d12	22.56

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
2			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4			Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	94
5			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.58	11.5	ng	157977	1	8.86	275593	20.0
2-Pentanone, 4-hy...	5.78	3.4	ng	46458	1	8.86	275593	20.0
unknown8.38	8.38	91.4	ng	1259830	1	8.86	275593	20.0
n-Hexadecanoic acid	19.02	3.1	ng	123835	4	18.21	805024	20.0
Pentafluoropropio...	22.07	2.9	ng	129183	5	22.56	896059	20.0