

Data Path : Z:\HPCHEM1\BNA G\DATA\BG121115\
Data File : BG020077.D
Acq On : 10 Dec 2015 15:59
Operator : UM/SJ
Sample : G4683-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S9-14.5

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-BG120215.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	2.990	21	26	46	rVB	1452019	2053347	100.00%	19.636%
2	5.182	390	399	407	rBV	75049	112218	5.47%	1.073%
3	5.658	471	480	491	rBV	353014	559219	27.23%	5.348%
4	7.262	744	753	767	rBV	387906	664122	32.34%	6.351%
5	7.638	809	817	827	rVB	367318	629382	30.65%	6.019%
6	8.108	891	897	903	rBV	66833	111783	5.44%	1.069%
7	8.437	945	953	960	rBV	263888	443474	21.60%	4.241%
8	9.277	1089	1096	1105	rBV	240640	412953	20.11%	3.949%
9	10.928	1368	1377	1385	rBV	98438	172590	8.41%	1.650%
10	13.366	1783	1792	1800	rBV	584405	918673	44.74%	8.785%
11	14.183	1924	1931	1939	rBV	130375	181431	8.84%	1.735%
12	14.741	2019	2026	2033	rVB2	161378	263878	12.85%	2.523%
13	16.222	2268	2278	2289	rBV	551963	820299	39.95%	7.844%
14	16.427	2307	2313	2320	rBV	16890	28451	1.39%	0.272%
15	17.479	2486	2492	2497	rBV2	230008	339529	16.54%	3.247%
16	18.349	2635	2640	2645	rBV2	56458	81101	3.95%	0.776%
17	19.524	2826	2840	2850	rBV	24981	47732	2.32%	0.456%
18	19.618	2852	2856	2863	rBV3	19401	30554	1.49%	0.292%
19	19.765	2875	2881	2885	rBV3	15769	30549	1.49%	0.292%
20	19.888	2897	2902	2907	rVB	35039	50690	2.47%	0.485%
21	20.082	2929	2935	2946	rVB	1165422	1509068	73.49%	14.431%
22	21.380	3151	3156	3168	rBV4	42980	89036	4.34%	0.851%
23	21.750	3211	3219	3225	rBV	271522	456637	22.24%	4.367%
24	23.977	3593	3598	3608	rBV6	7058	21572	1.05%	0.206%
25	24.077	3610	3615	3623	rVB6	9323	23066	1.12%	0.221%
26	25.029	3765	3777	3788	rBV2	144315	405861	19.77%	3.881%

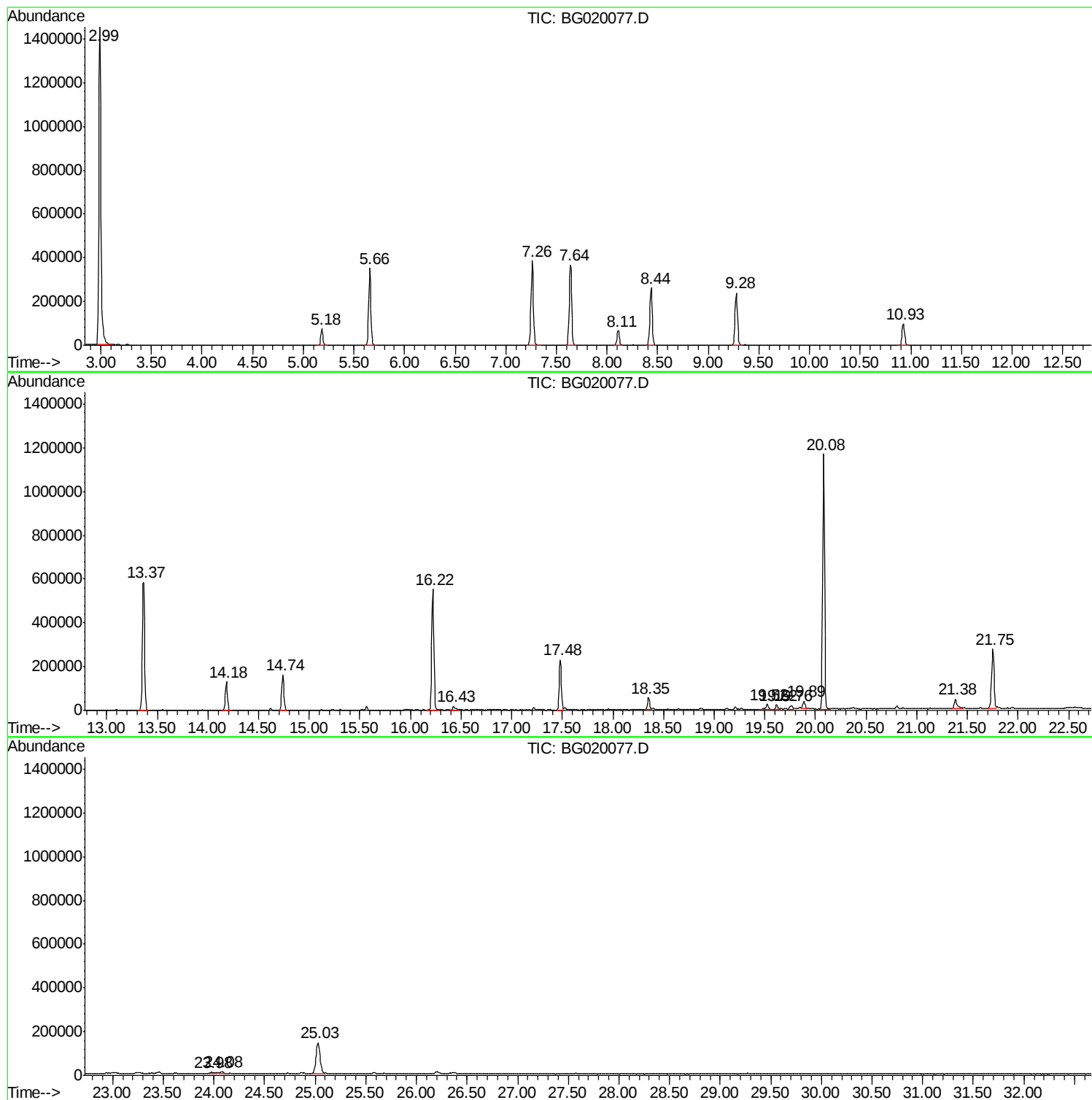
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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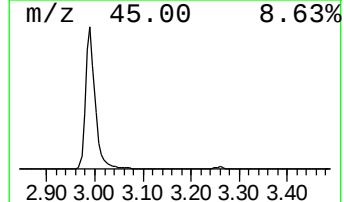
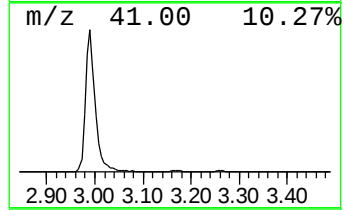
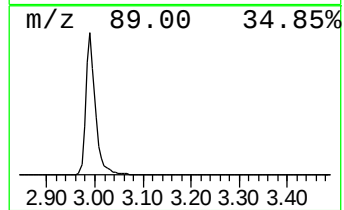
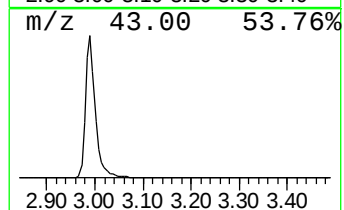
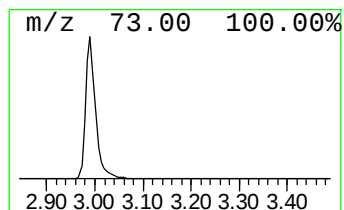
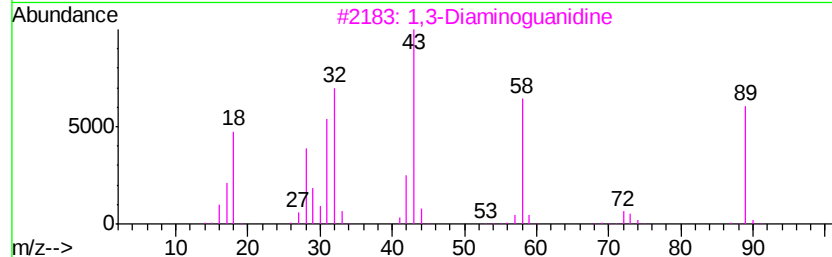
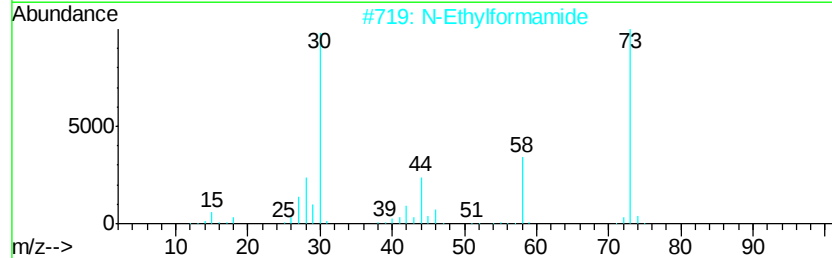
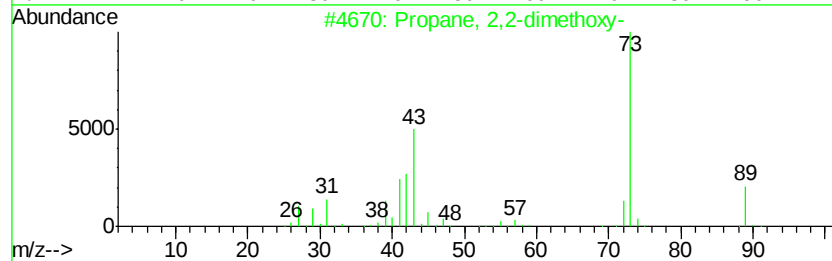
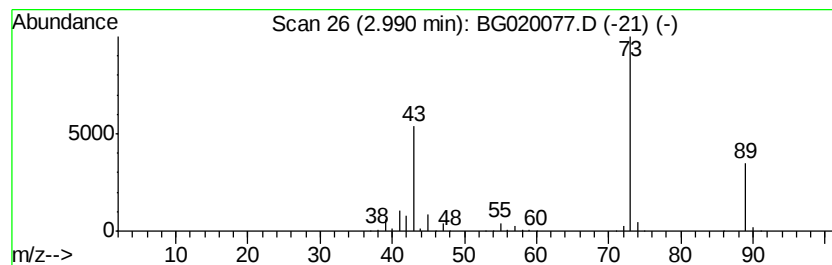
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	367.38 ng	2053350	1,4-Dichlorobenzene-d4	8.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2		N-Ethylformamide	73	C3H7NO	000627-45-2	9
3		1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5		1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9



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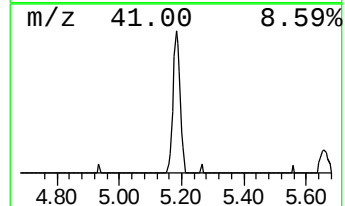
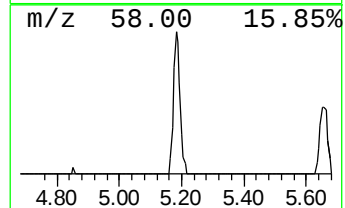
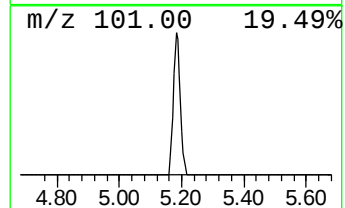
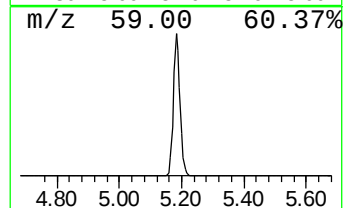
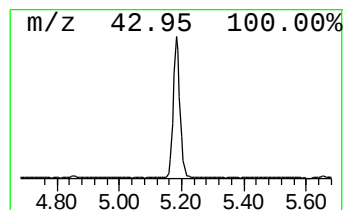
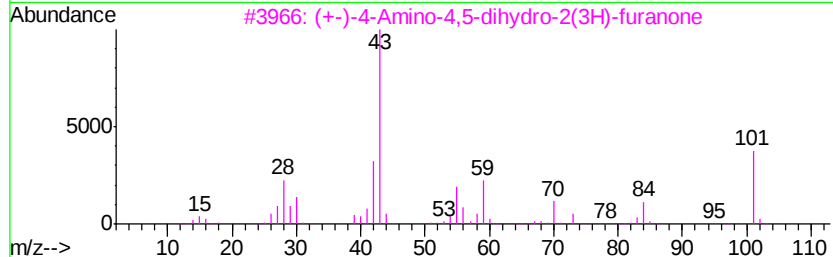
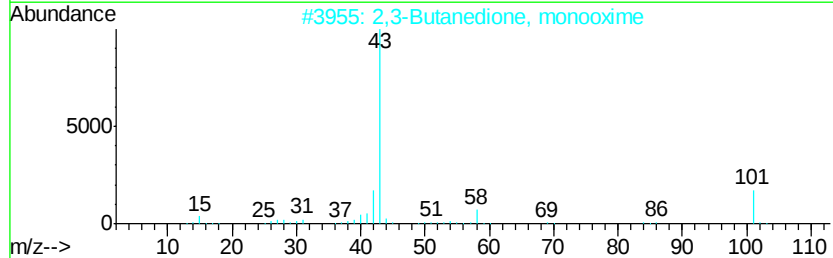
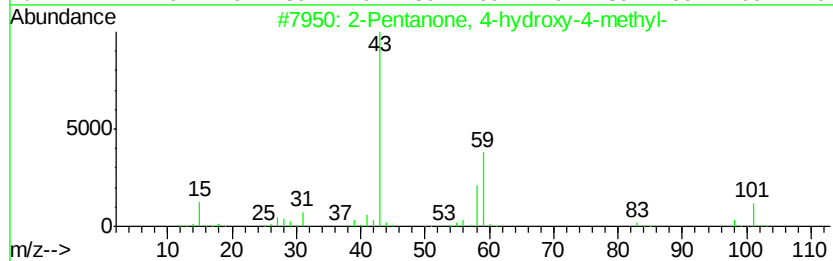
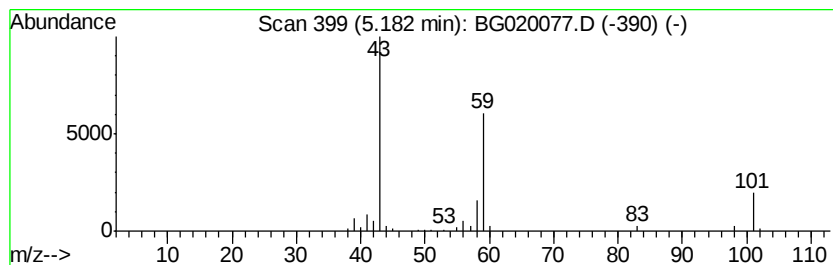
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	20.08 ng	112218	1,4-Dichlorobenzene-d4	8.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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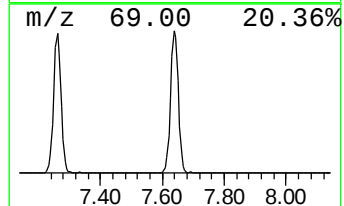
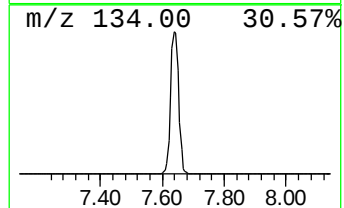
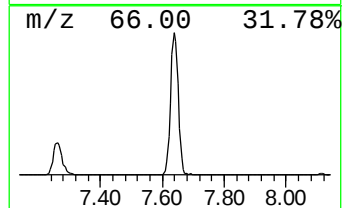
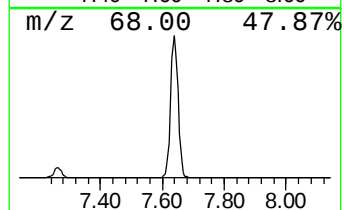
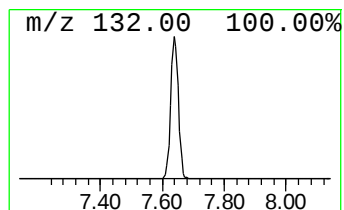
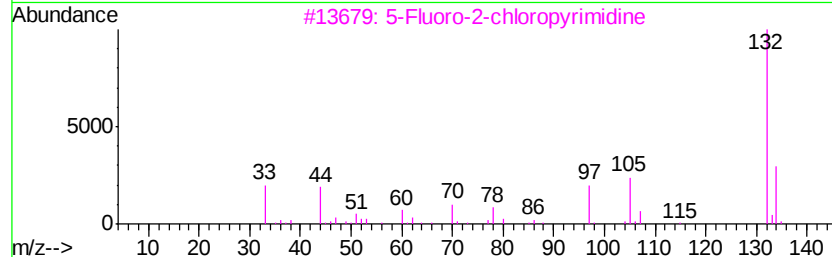
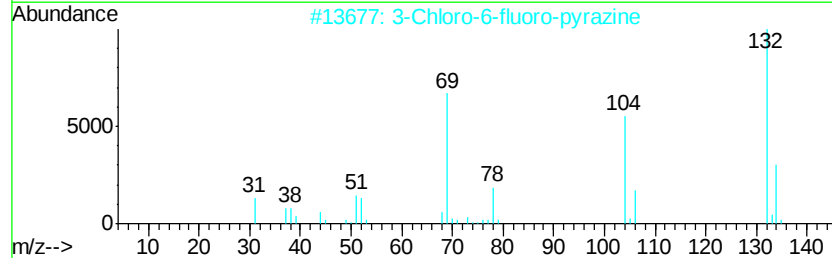
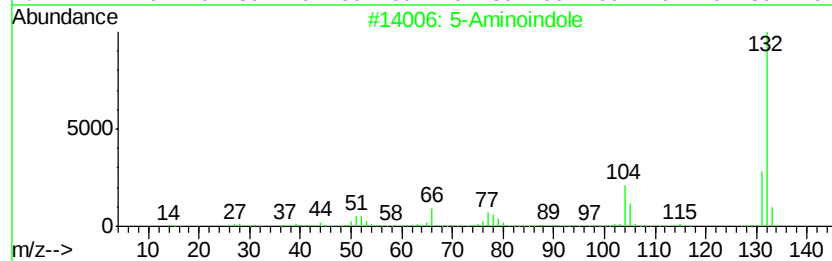
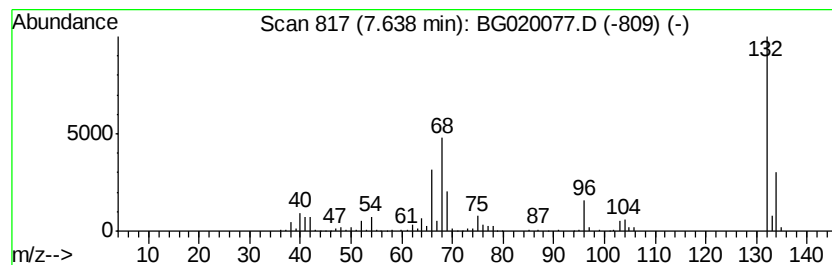
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Peak Number 3 unknown7.64 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	112.61 ng	629382	1,4-Dichlorobenzene-d4	8.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	22
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		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



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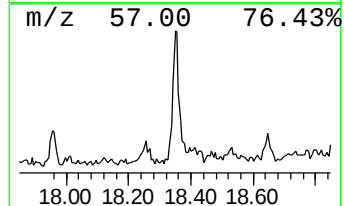
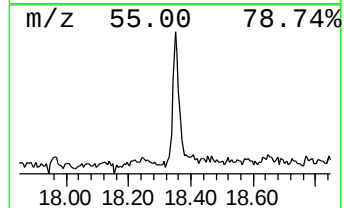
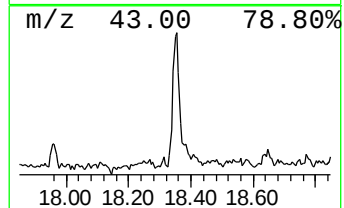
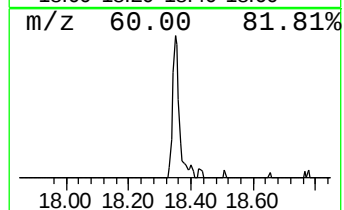
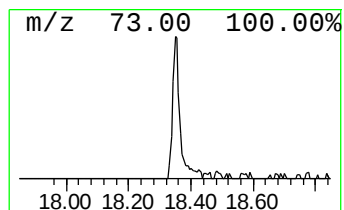
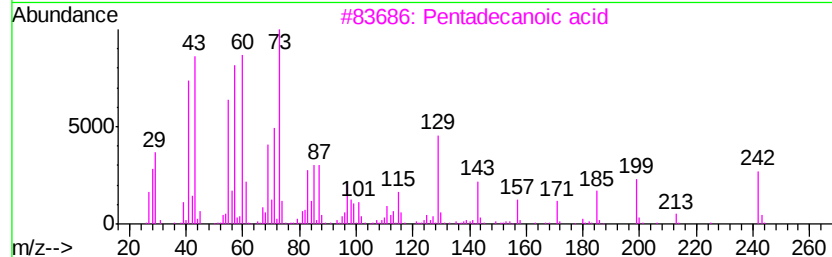
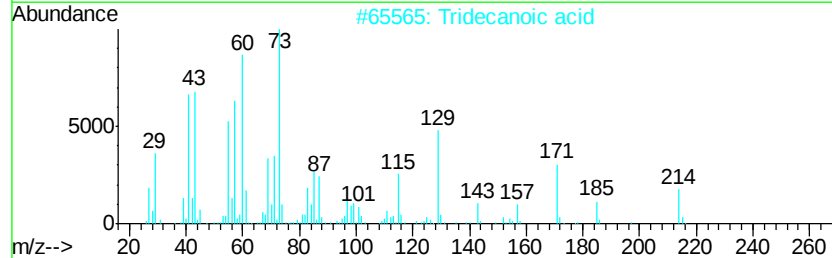
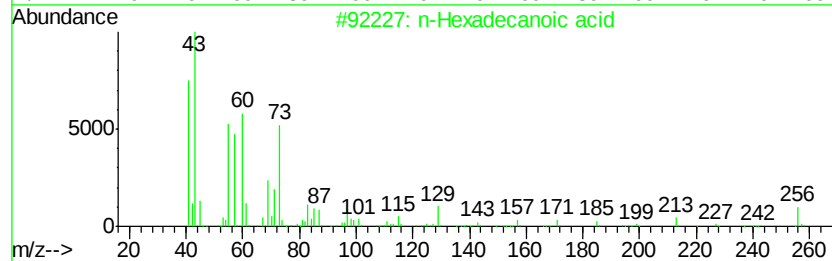
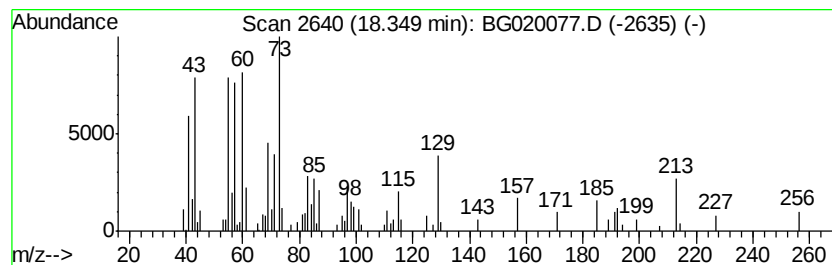
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.35	4.78 ng	81101	Phenanthrene-d10		17.48
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Dodecanoic acid	200	C12H24O2	000143-07-7	47



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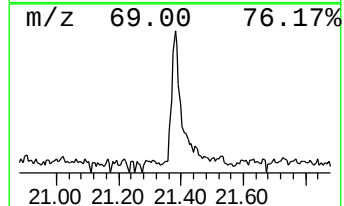
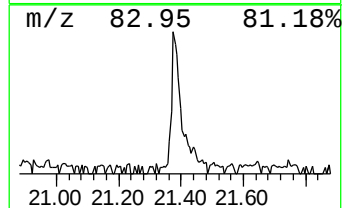
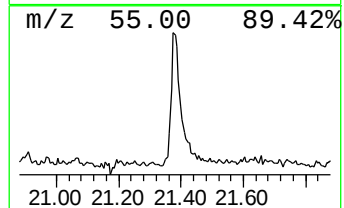
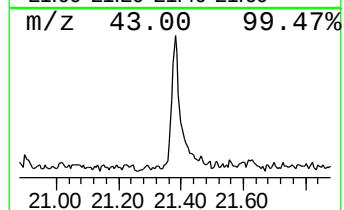
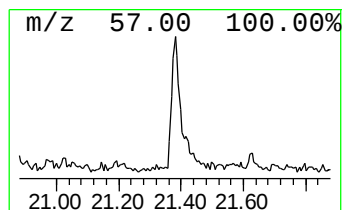
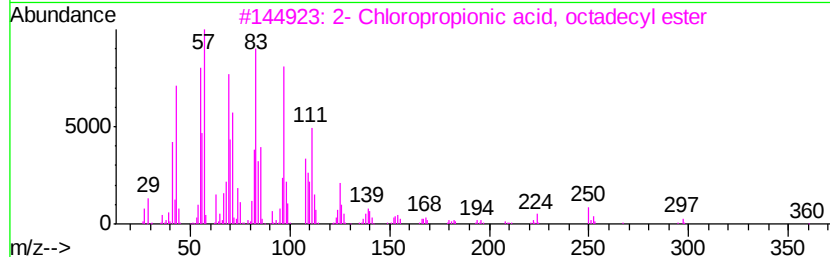
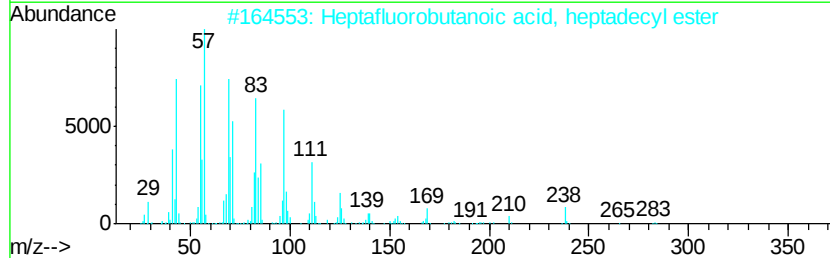
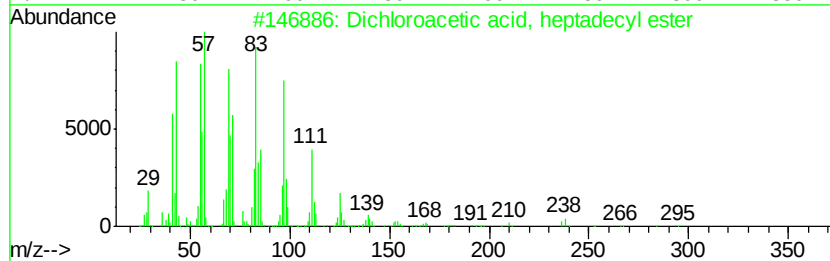
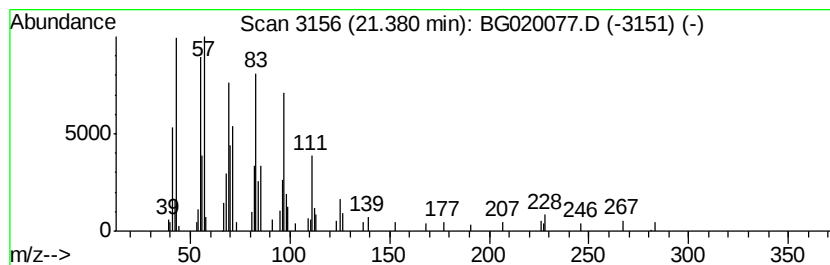
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Peak Number 8 Dichloroacetic acid, heptad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.38	3.90 ng	89036	Chrysene-d12	21.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94
3		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
4		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	2.99	367.4	ng	2053350	1	8.11	111783	20.0
2-Pentanone, 4-hy...	5.18	20.1	ng	112218	1	8.11	111783	20.0
unknown7.64	7.64	112.6	ng	629382	1	8.11	111783	20.0
n-Hexadecanoic acid	18.35	4.8	ng	81101	4	17.48	339529	20.0
Dichloroacetic ac...	21.38	3.9	ng	89036	5	21.75	456637	20.0