

Data Path : Z:\HPCHEM1\BNA G\DATA\BG031318\
 Data File : BG033117.D
 Acq On : 13 Mar 2018 13:21
 Operator : SJ/JU
 Sample : J1873-09
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-9B-COMP

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-BG022118.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	3.517	32	39	51	rVB3	26932	73558	3.89%	0.555%
2	5.819	425	431	442	rVB2	19658	34146	1.81%	0.258%
3	6.324	510	517	528	rBV	632443	1092023	57.77%	8.243%
4	8.005	794	803	820	rBV	643112	1181210	62.49%	8.916%
5	8.422	865	874	889	rBV	618423	1135231	60.06%	8.569%
6	8.909	950	957	970	rVB	169159	298310	15.78%	2.252%
7	9.250	1006	1015	1023	rBV	432275	811206	42.92%	6.123%
8	10.108	1153	1161	1169	rBV	365170	692648	36.64%	5.228%
9	11.794	1441	1448	1458	rBV	238398	436882	23.11%	3.298%
10	14.149	1840	1849	1859	rBV	883123	1426070	75.44%	10.764%
11	14.942	1977	1984	1989	rBV	68392	98353	5.20%	0.742%
12	15.353	2048	2054	2059	rBV	21961	29510	1.56%	0.223%
13	15.524	2076	2083	2095	rVB2	333313	551739	29.19%	4.165%
14	16.287	2209	2213	2218	rVB	27774	35033	1.85%	0.264%
15	16.992	2326	2333	2346	rBV	681794	1065896	56.39%	8.046%
16	17.145	2354	2359	2368	rVB	22643	36187	1.91%	0.273%
17	18.250	2540	2547	2557	rBV	419445	654399	34.62%	4.940%
18	19.048	2678	2683	2691	rBV2	66898	102516	5.42%	0.774%
19	20.764	2969	2975	2984	rBV	1432272	1890226	100.00%	14.268%
20	22.121	3201	3206	3226	rBV4	65758	191813	10.15%	1.448%
21	22.602	3281	3288	3301	rBV2	371359	710568	37.59%	5.364%
22	24.506	3604	3612	3618	rBV3	18089	36547	1.93%	0.276%
23	26.397	3922	3934	3948	rBV2	186452	664122	35.13%	5.013%

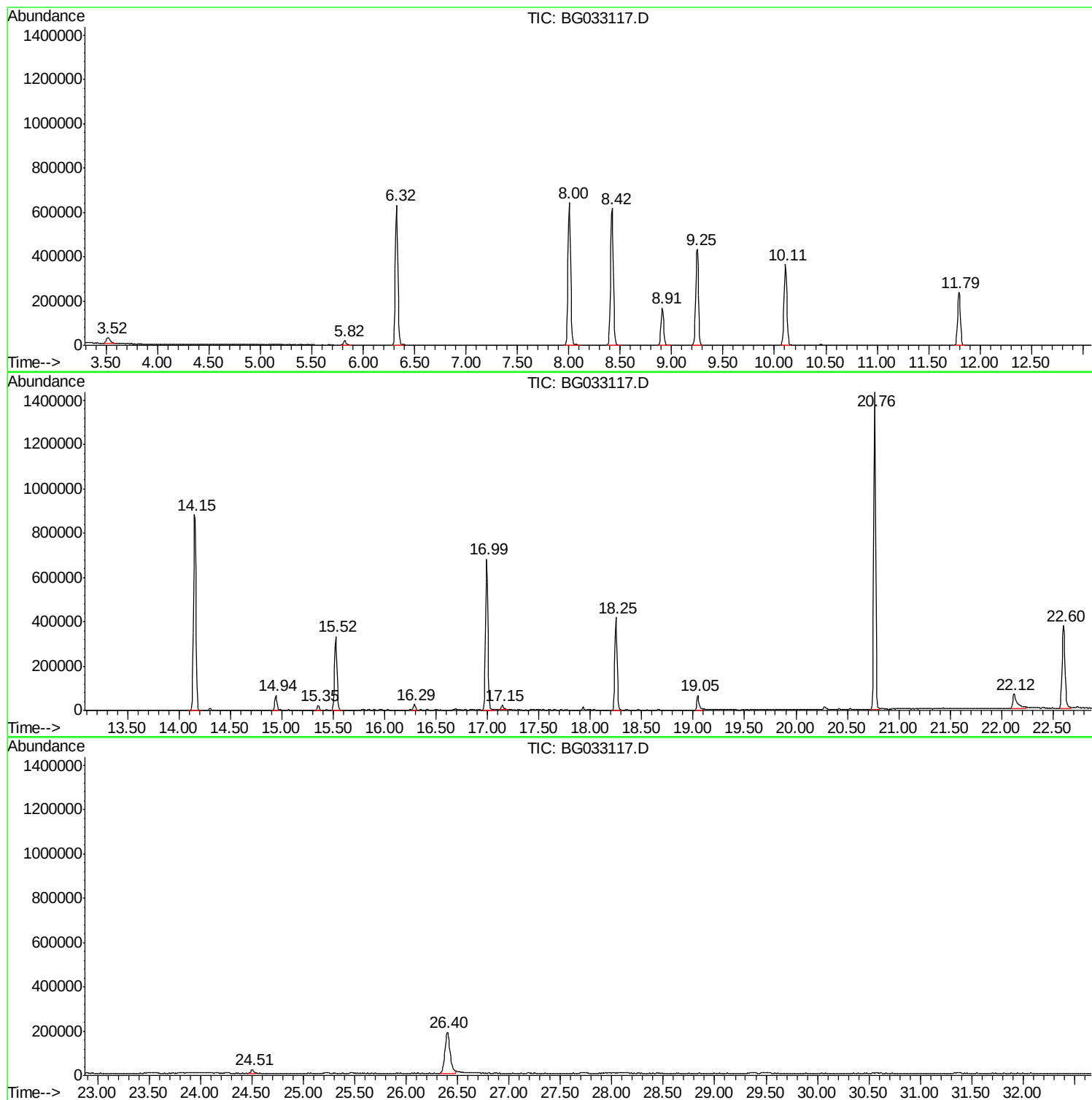
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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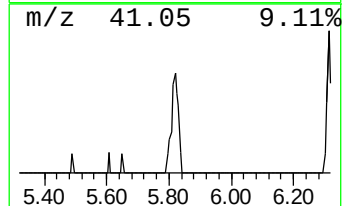
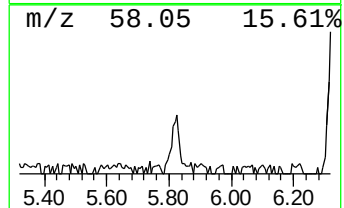
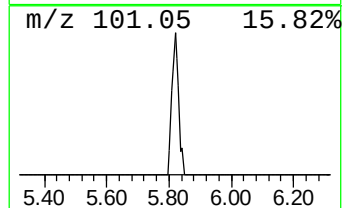
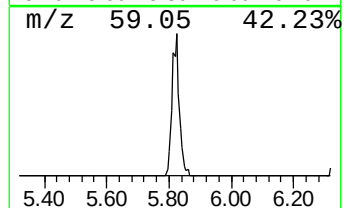
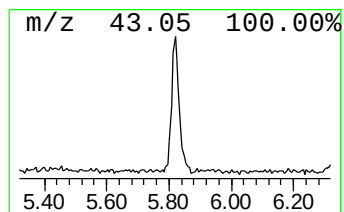
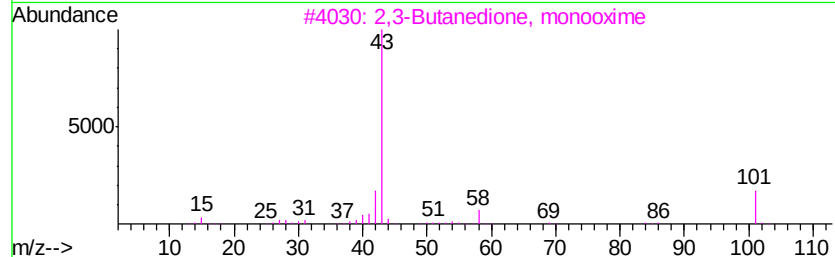
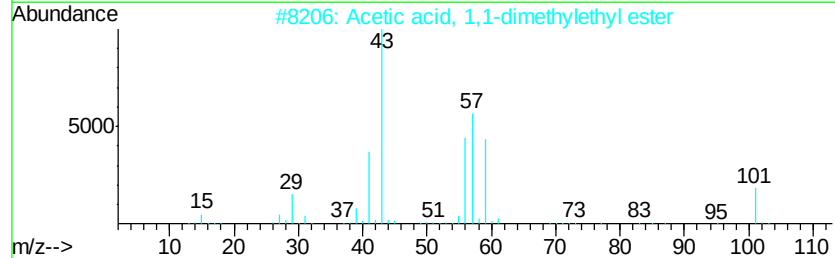
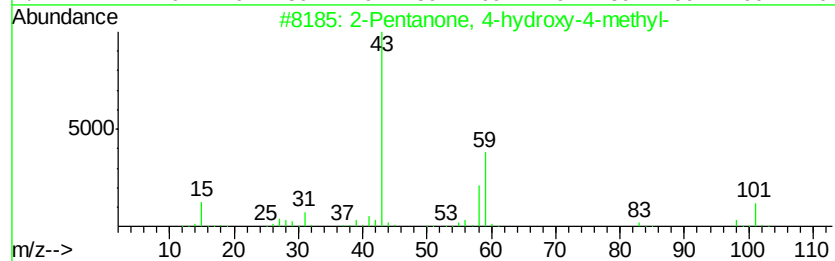
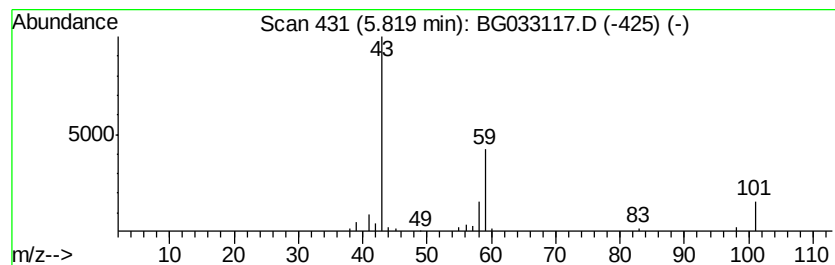
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG022118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.82	2.29 ng	34146	1,4-Dichlorobenzene-d4	8.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	78
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5		Butanoic acid, 4-amino-3-hydroxy...	119	C4H9NO3	000924-49-2	9



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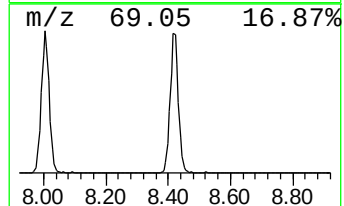
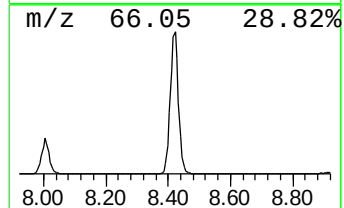
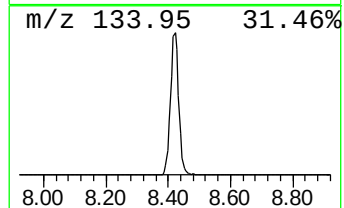
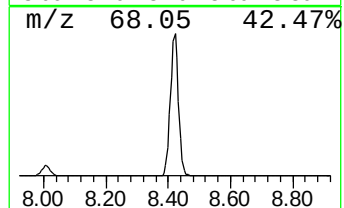
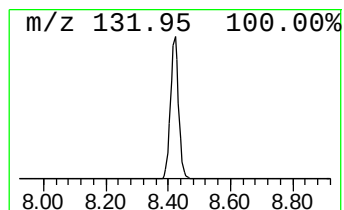
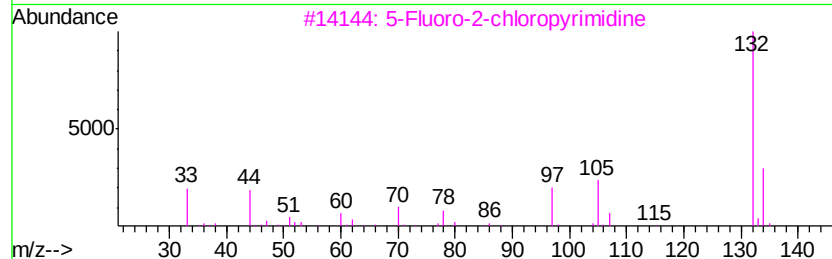
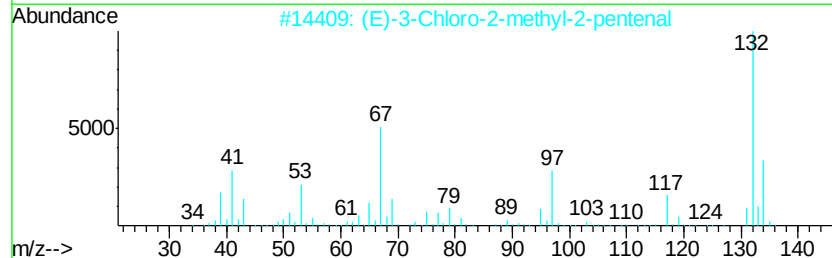
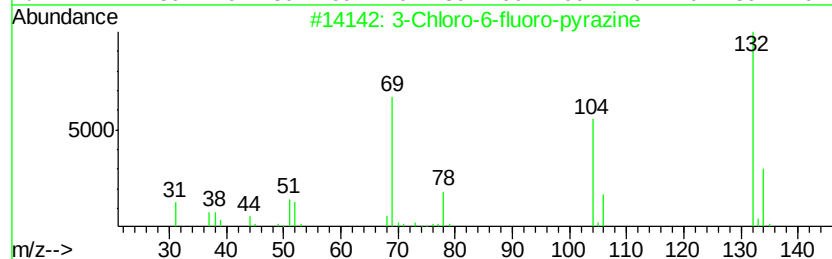
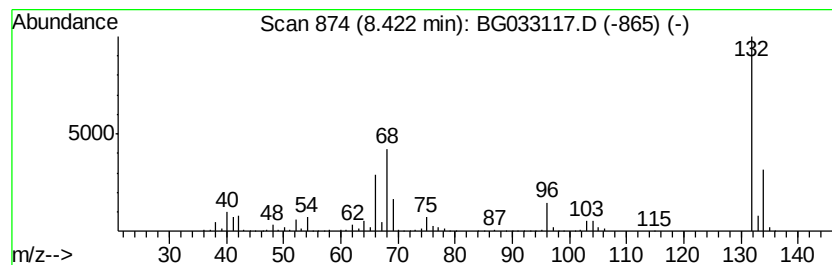
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Peak Number 3 unknown8.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.42	76.11 ng	1135230	1,4-Dichlorobenzene-d4	8.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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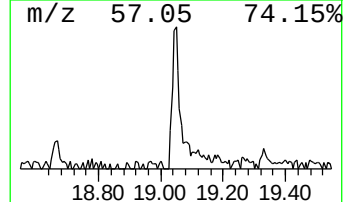
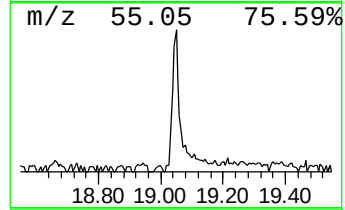
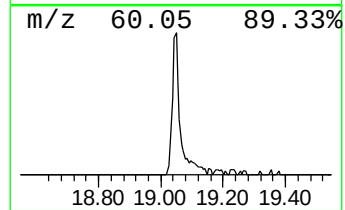
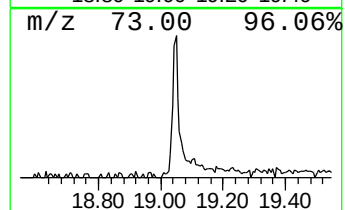
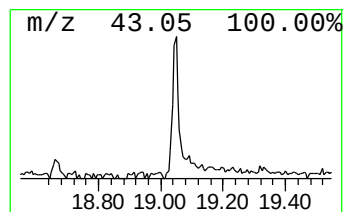
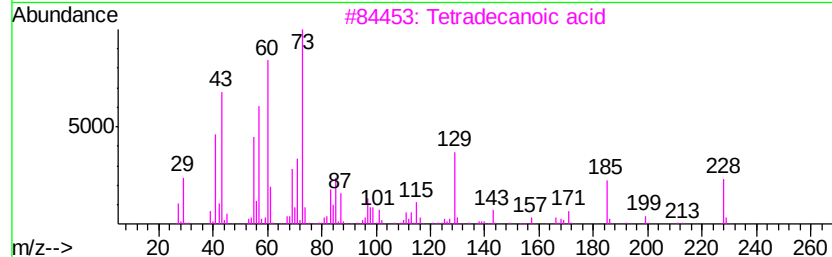
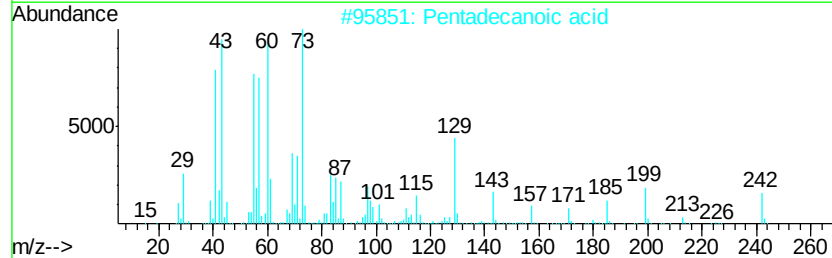
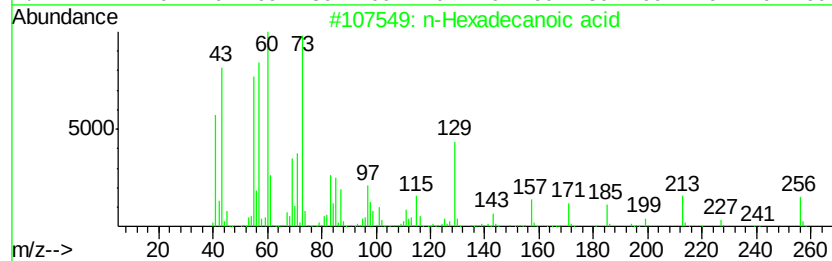
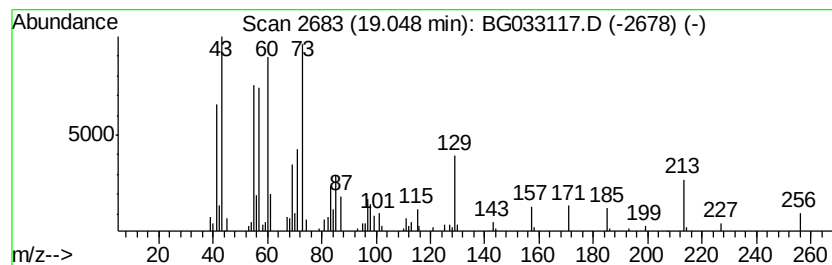
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
19.05	3.13 ng	102516	Phenanthrene-d10		18.25
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	Undecanoic acid	186	C11H22O2	000112-37-8	62



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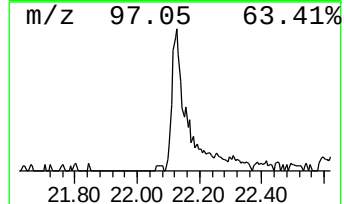
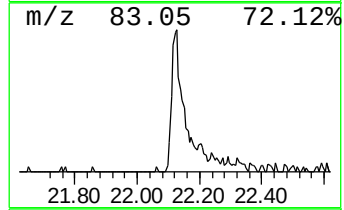
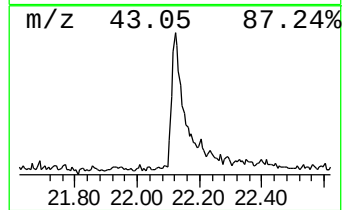
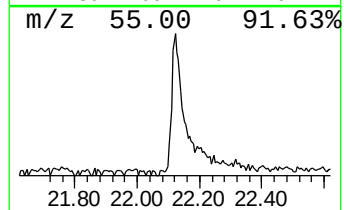
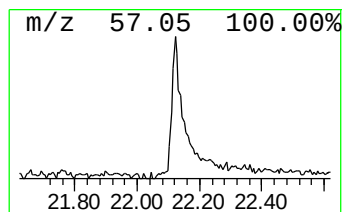
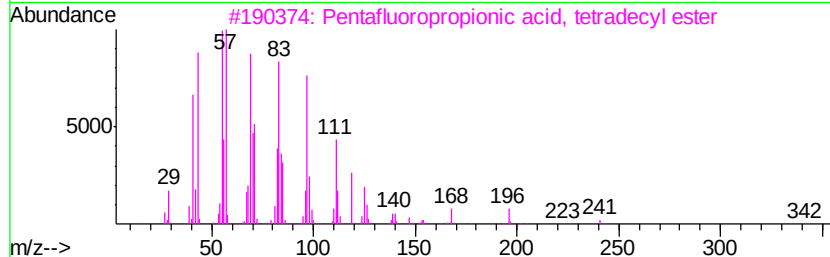
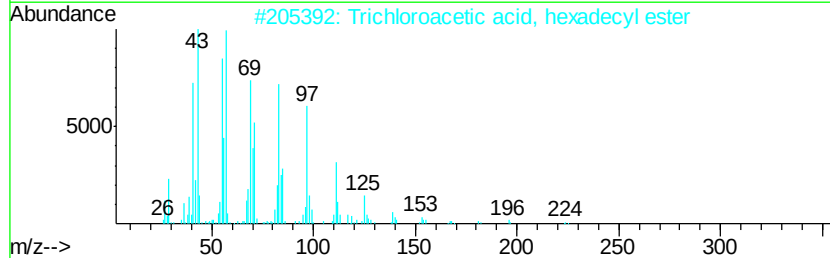
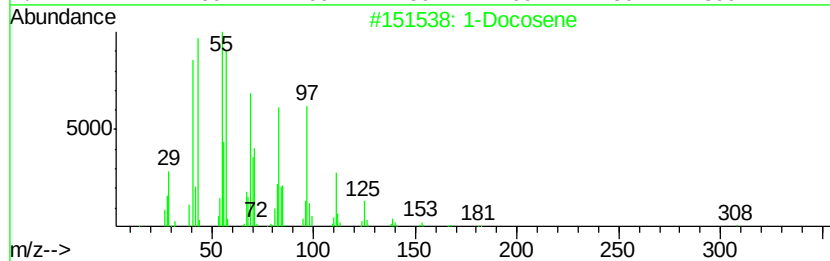
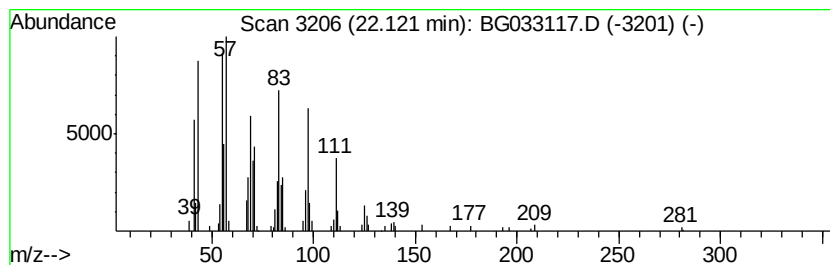
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Peak Number 6 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.12	5.40 ng	191813	Chrysene-d12	22.60
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Docosene		308 C22H44	001599-67-3 94
2	Trichloroacetic acid, hexadecyl ...		386 C18H33Cl3O2	074339-54-1 93
3	Pentafluoropropionic acid, tetra...		360 C17H29F5O2	006222-06-6 91
4	Pentafluoropropionic acid, penta...		374 C18H31F5O2	959092-08-1 91
5	2- Chloropropionic acid, pentade...		318 C18H35ClO2	1000292-44-1 91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.82	2.3	ng	34146	1	8.91	298310	20.0
unknown8.42	8.42	76.1	ng	1135230	1	8.91	298310	20.0
n-Hexadecanoic acid	19.05	3.1	ng	102516	4	18.25	654399	20.0
1-Docosene	22.12	5.4	ng	191813	5	22.60	710568	20.0