

Data Path : Z:\HPCHEM1\BNA G\DATA\BG042018\
 Data File : BG033884.D
 Acq On : 20 Apr 2018 13:46
 Operator : SJ/JU
 Sample : J2455-11
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-2

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-BG041918.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	4.998	286	291	301	rVB	129091	197502	4.06%	0.668%
2	5.444	358	367	377	rBV	1439736	2304060	47.39%	7.789%
3	7.007	624	633	644	rBV	1468776	2630780	54.11%	8.893%
4	7.371	687	695	704	rBV	1474197	2444113	50.27%	8.262%
5	7.836	765	774	781	rBV	291071	467855	9.62%	1.582%
6	8.153	820	828	838	rBV	1029600	1762966	36.26%	5.960%
7	8.987	960	970	981	rBV	837952	1493079	30.71%	5.047%
8	10.621	1240	1248	1255	rBV	378125	675870	13.90%	2.285%
9	13.094	1661	1669	1677	rVB	2121724	3305695	67.99%	11.175%
10	13.928	1805	1811	1817	rBV	281735	403727	8.30%	1.365%
11	14.469	1895	1903	1911	rVV2	591833	963596	19.82%	3.257%
12	15.350	2048	2053	2058	rVB	54046	68344	1.41%	0.231%
13	15.955	2149	2156	2166	rVB	1865272	2826157	58.13%	9.554%
14	16.214	2195	2200	2204	rBV	49024	65023	1.34%	0.220%
15	17.219	2364	2371	2377	rBV	837875	1228924	25.28%	4.154%
16	18.141	2522	2528	2545	rBV	278786	485729	9.99%	1.642%
17	19.422	2742	2746	2757	rBV2	107303	187576	3.86%	0.634%
18	19.857	2814	2820	2826	rBV	3670193	4861959	100.00%	16.436%
19	21.179	3038	3045	3060	rBV	170431	346124	7.12%	1.170%
20	21.478	3089	3096	3104	rVB	906699	1439354	29.60%	4.866%
21	24.545	3602	3618	3630	rBV2	532190	1423345	29.28%	4.812%

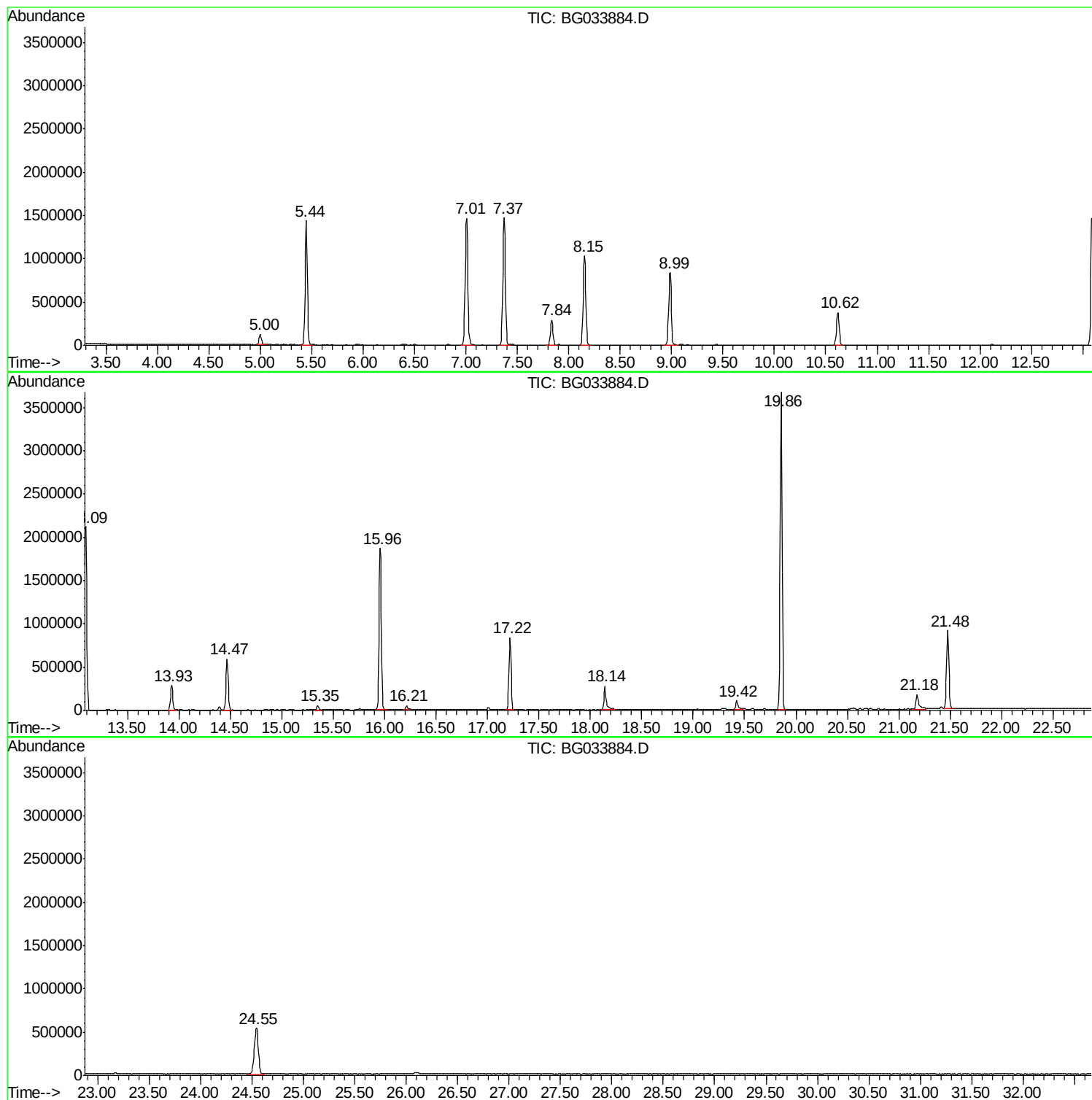
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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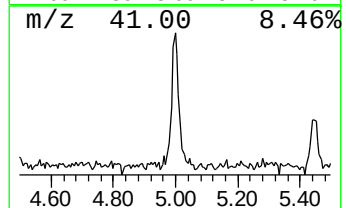
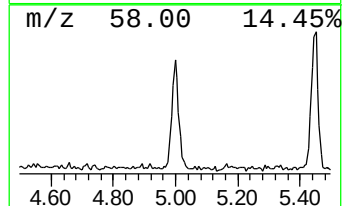
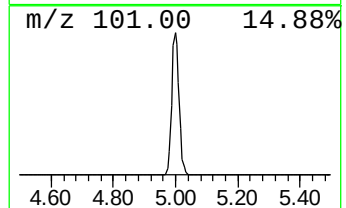
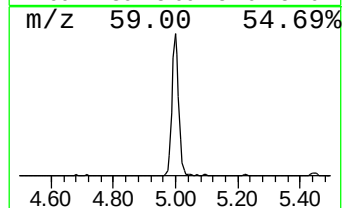
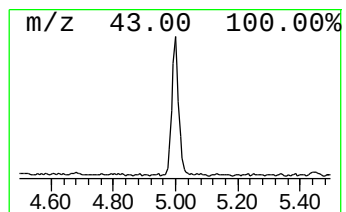
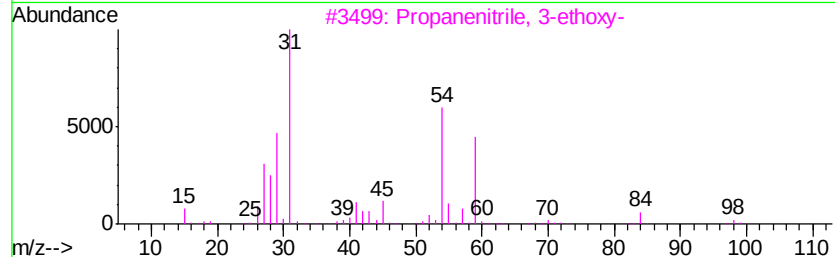
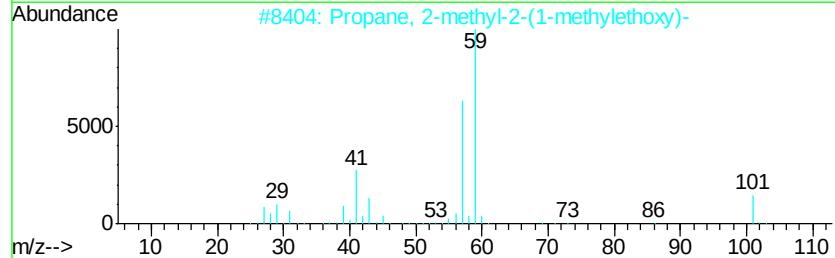
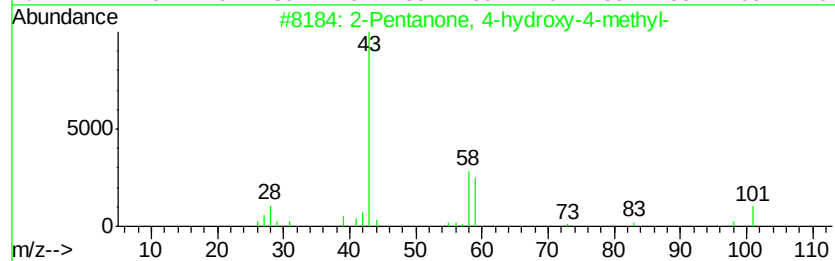
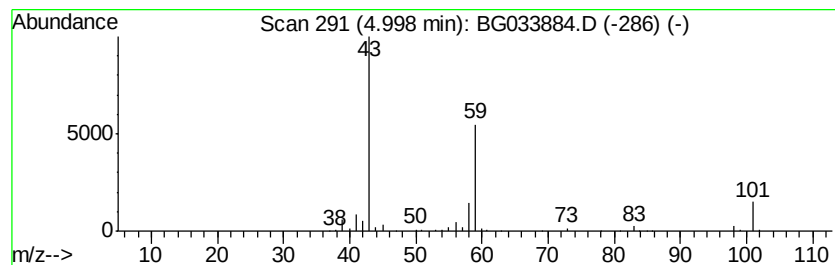
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	8.44 ng	197502	1,4-Dichlorobenzene-d4	7.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3		Propanenitrile, 3-ethoxy-	99	C5H9NO	002141-62-0	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		3-Hexanol	102	C6H14O	000623-37-0	9



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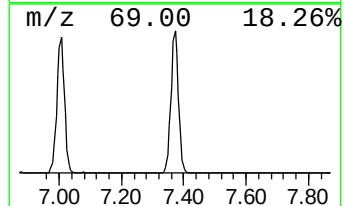
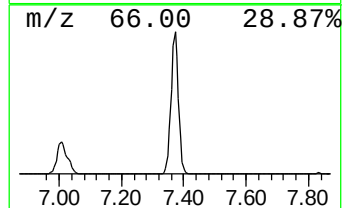
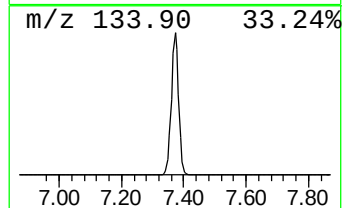
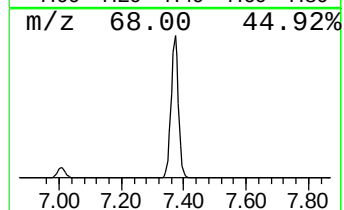
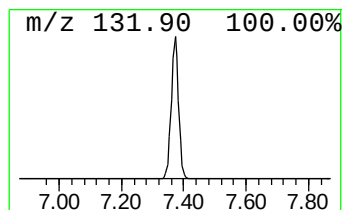
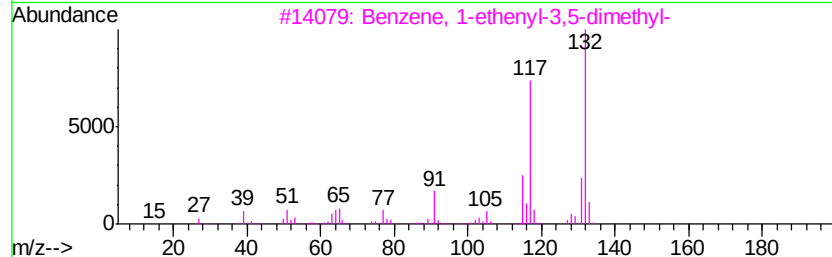
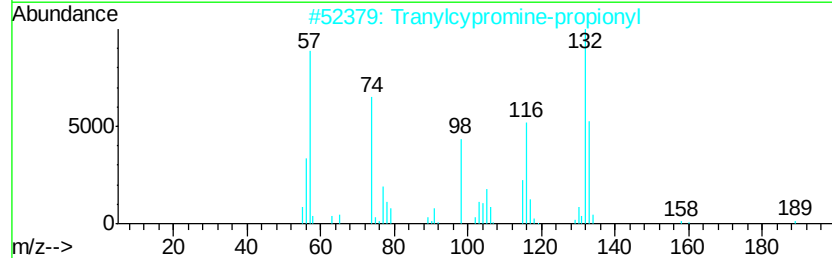
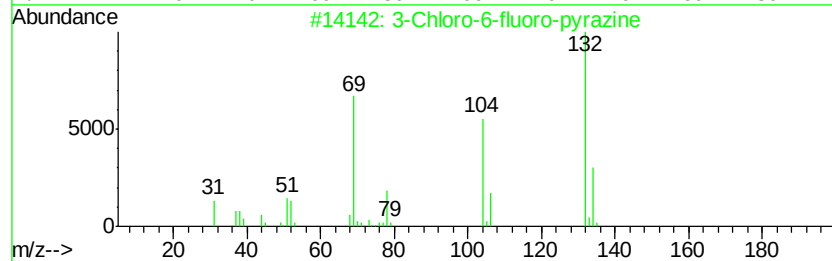
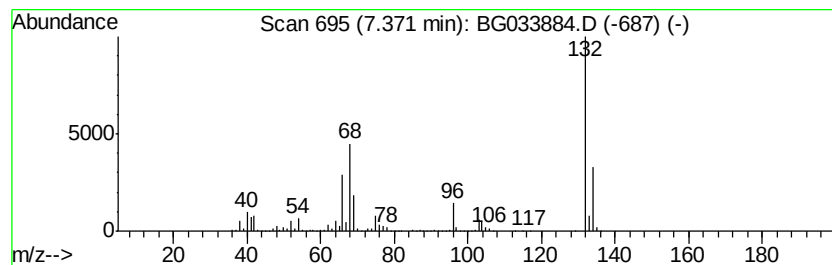
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Peak Number 2 unknown7.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.37	104.48 ng	2444110	1,4-Dichlorobenzene-d4	7.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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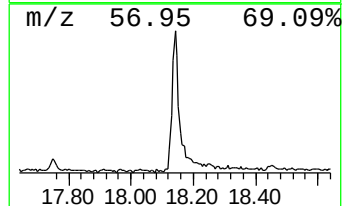
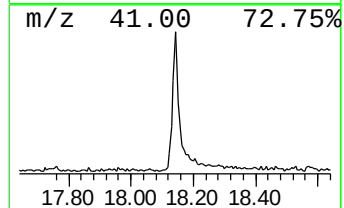
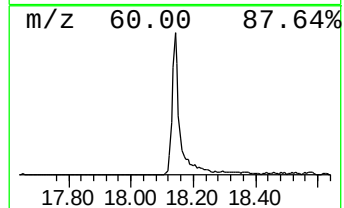
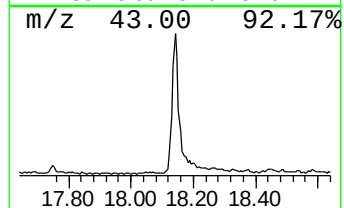
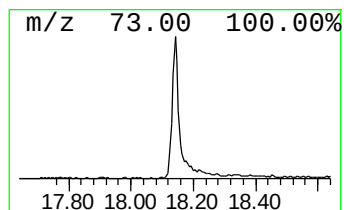
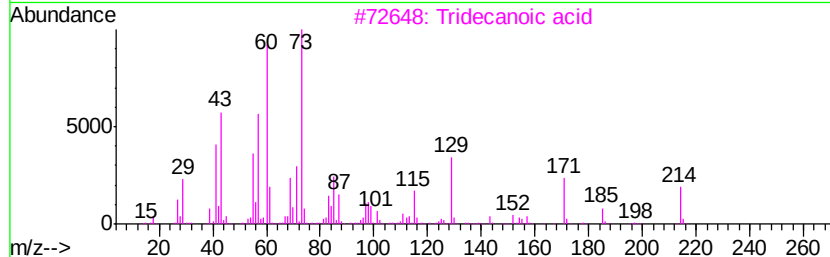
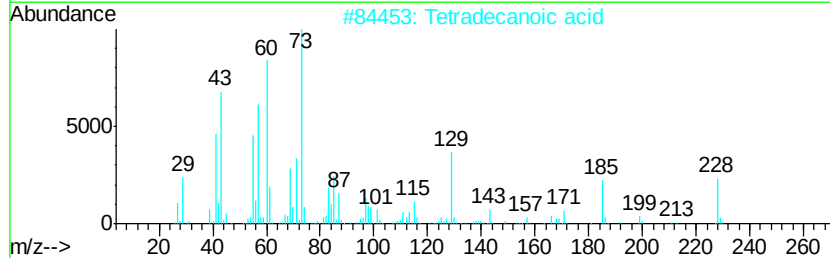
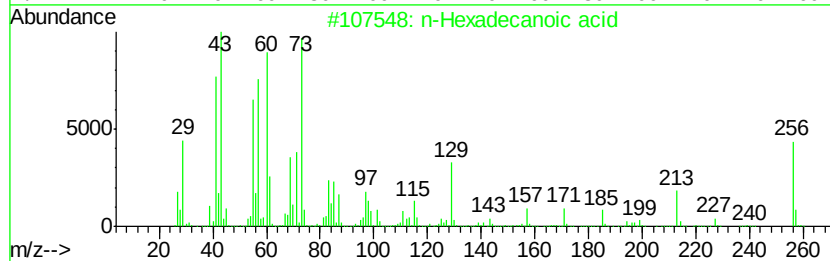
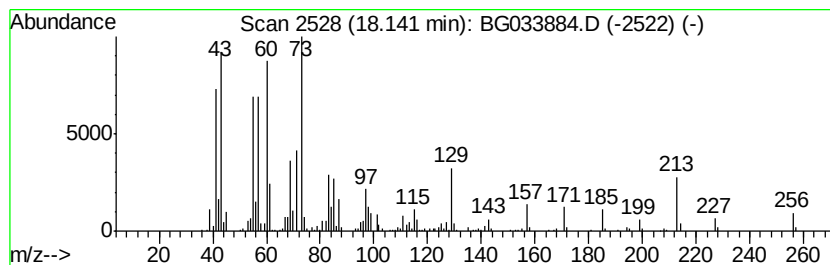
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.14	7.90 ng	485729	Phenanthrene-d10	17.22

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3		Tridecanoic acid	214	C13H26O2	000638-53-9	91
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	62
5		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	58



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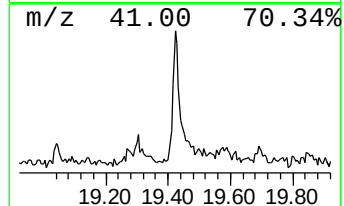
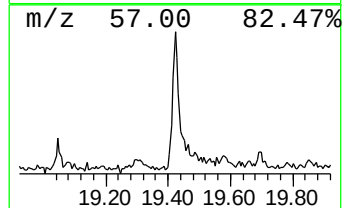
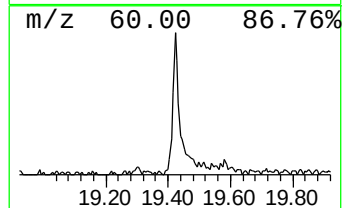
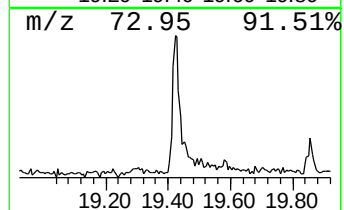
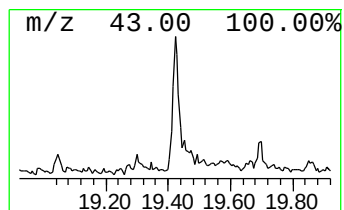
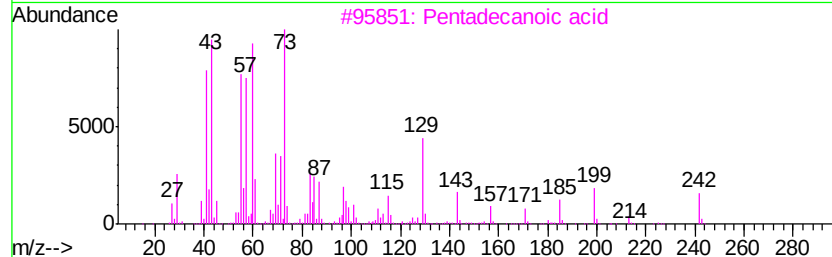
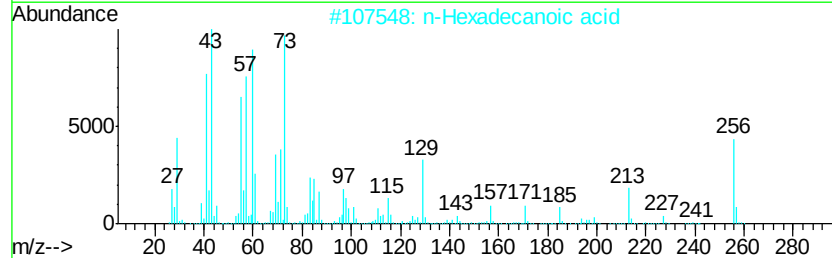
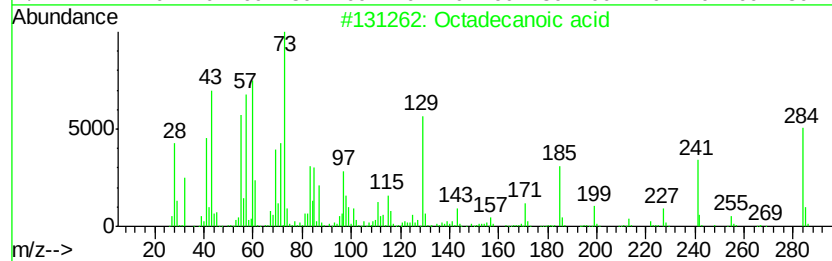
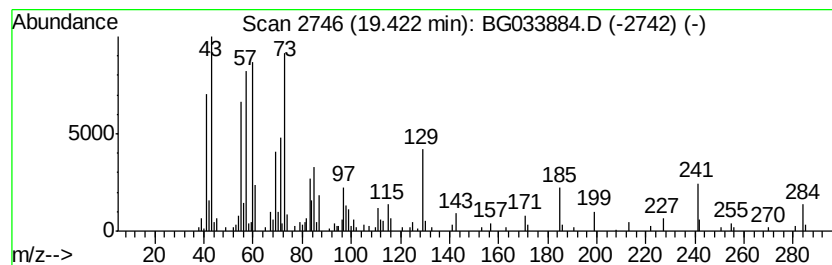
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Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
19.42	2.61 ng	187576	Chrysene-d12		21.48
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4	Heptadecanoic acid	270	C17H34O2	000506-12-7	80
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74



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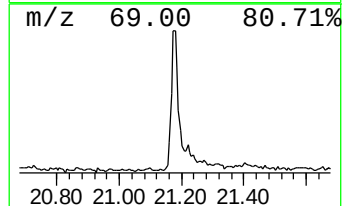
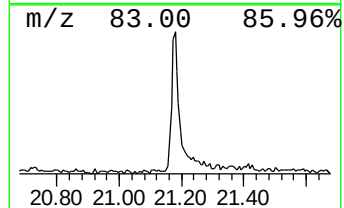
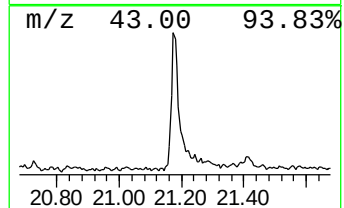
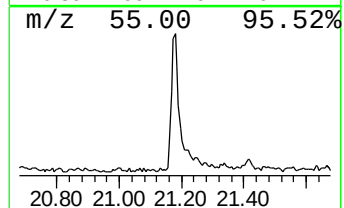
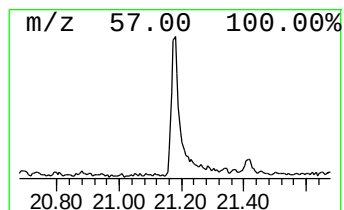
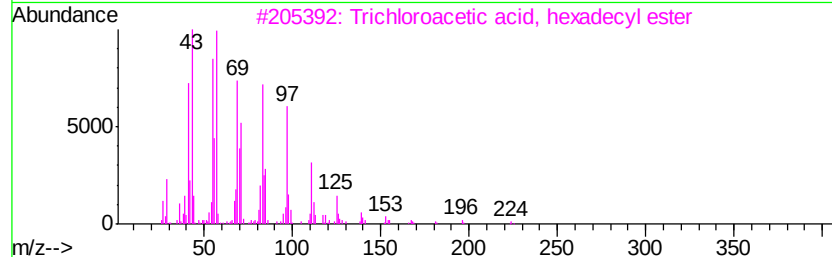
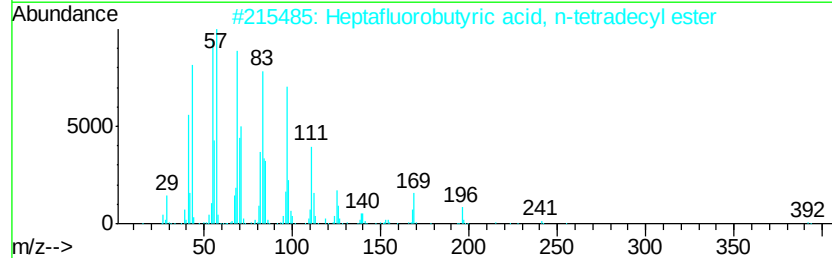
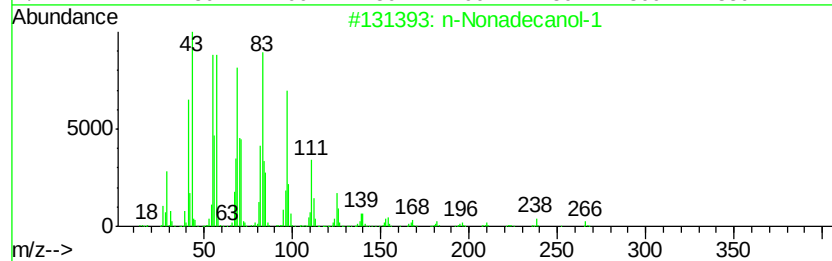
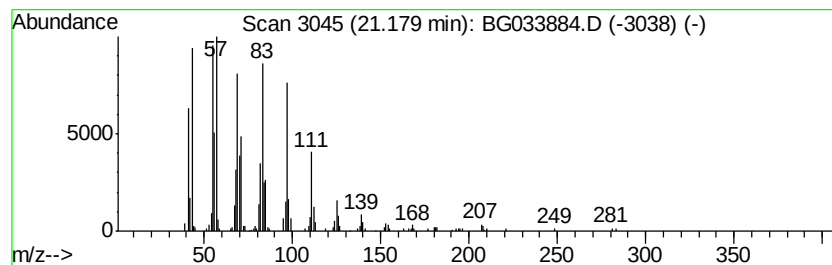
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Peak Number 6 n-Nonadecanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.18	4.81 ng	346124	Chrysene-d12	21.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	n-Nonadecanol-1	284 C19H40O	001454-84-8	95
2	Heptafluorobutyric acid, n-tetra...	410 C18H29F7O2	007365-36-8	94
3	Trichloroacetic acid, hexadecyl ...	386 C18H33Cl3O2	074339-54-1	94
4	Trichloroacetic acid, pentadecyl...	372 C17H31Cl3O2	074339-53-0	94
5	Trifluoroacetic acid, pentadecyl...	324 C17H31F3O2	959010-23-2	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.00	8.4	ng	197502	1	7.84	467855	20.0
unknown7.37	7.37	104.5	ng	2444110	1	7.84	467855	20.0
n-Hexadecanoic acid	18.14	7.9	ng	485729	4	17.22	1228920	20.0
Octadecanoic acid	19.42	2.6	ng	187576	5	21.48	1439350	20.0
n-Nonadecanol-1	21.18	4.8	ng	346124	5	21.48	1439350	20.0