

Data Path : Z:\HPCHEM1\BNA G\DATA\BG112117\
 Data File : BG031166.D
 Acq On : 21 Nov 2017 23:35
 Operator : SJ/JU
 Sample : I6505-05
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 LW-D

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-BG111017.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	5.694	403	409	429	rBV	465478	834063	15.30%	3.638%
2	7.304	676	683	703	rBV	297449	568395	10.43%	2.479%
3	7.668	737	745	760	rBV	903764	1651768	30.30%	7.204%
4	8.138	814	825	832	rBV	202565	355650	6.52%	1.551%
5	8.462	873	880	895	rBV	825084	1493064	27.39%	6.512%
6	9.308	1015	1024	1039	rBV	638594	1237968	22.71%	5.400%
7	9.760	1094	1101	1110	rBV2	49462	110952	2.04%	0.484%
8	10.953	1296	1304	1312	rBV	270561	528796	9.70%	2.306%
9	11.787	1437	1446	1453	rBV5	24598	74282	1.36%	0.324%
10	13.379	1710	1717	1732	rVB	2054587	3270116	59.99%	14.263%
11	14.754	1945	1951	1959	rBV2	476712	787537	14.45%	3.435%
12	16.241	2198	2204	2213	rBV	1655158	2617744	48.02%	11.418%
13	17.498	2412	2418	2424	rBV2	670153	1029823	18.89%	4.492%
14	18.368	2562	2566	2574	rBV4	79484	128815	2.36%	0.562%
15	19.625	2777	2780	2791	rBV5	83669	147955	2.71%	0.645%
16	20.089	2853	2859	2866	rBV	4055242	5451373	100.00%	23.777%
17	21.770	3139	3145	3153	rVB	788011	1330427	24.41%	5.803%
18	25.072	3697	3707	3722	rVB2	452341	1308246	24.00%	5.706%

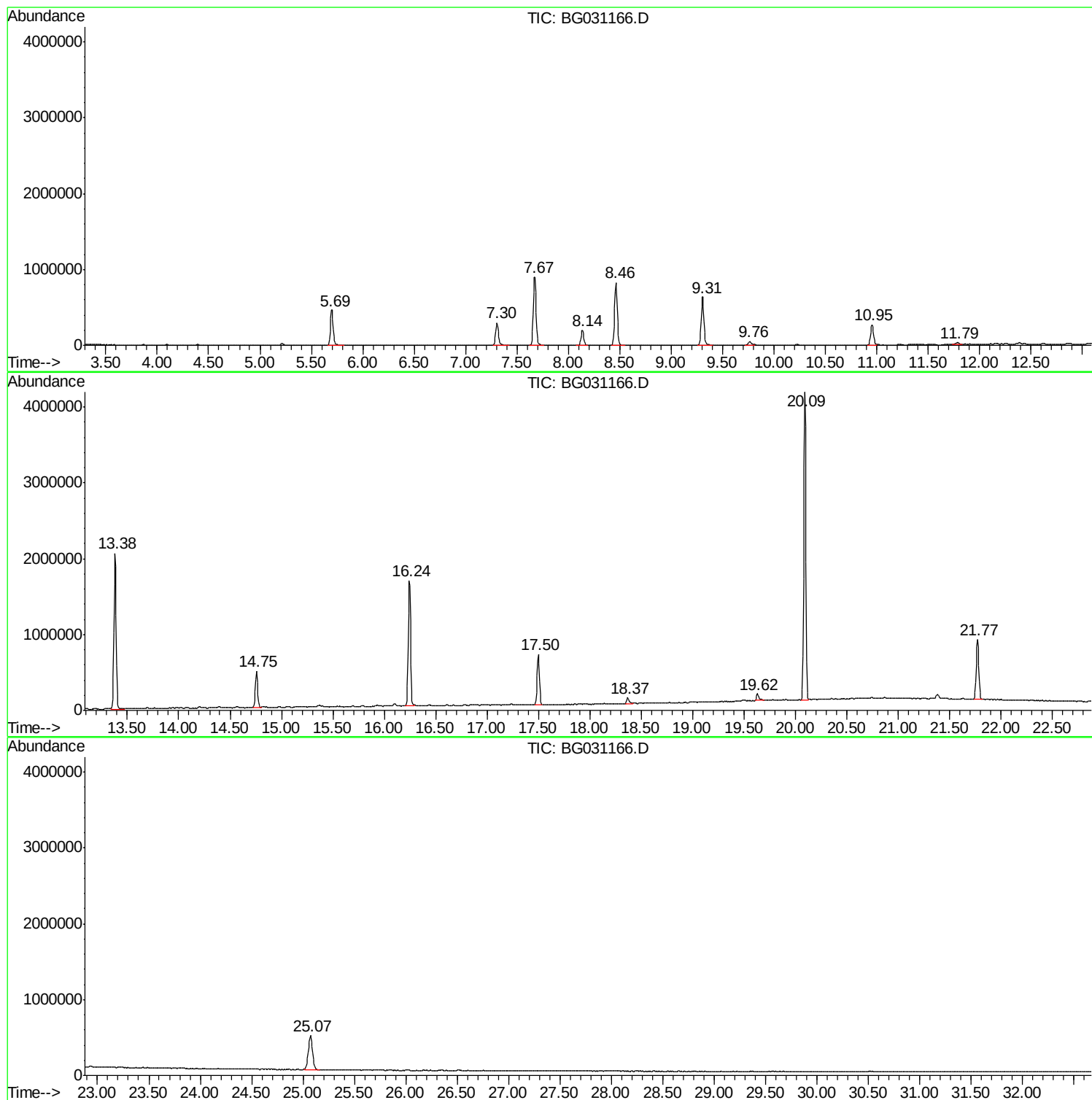
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG111017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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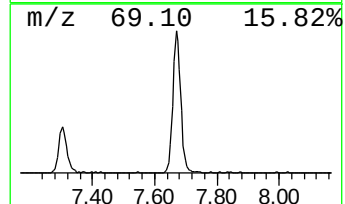
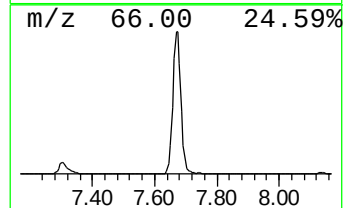
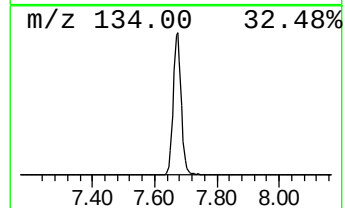
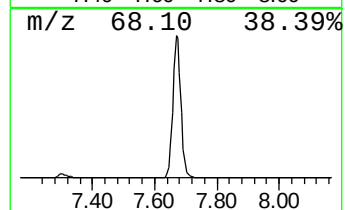
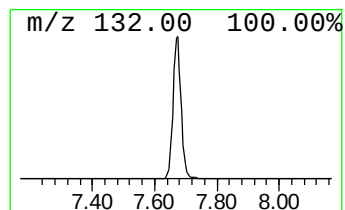
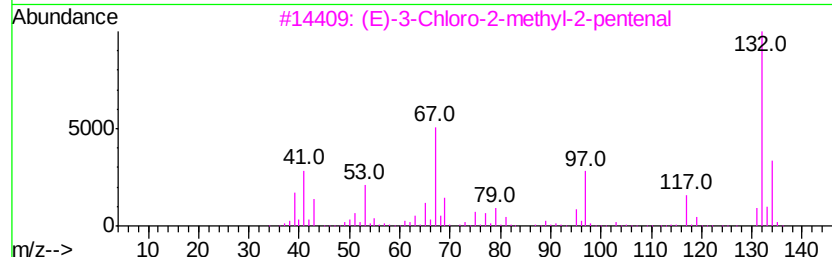
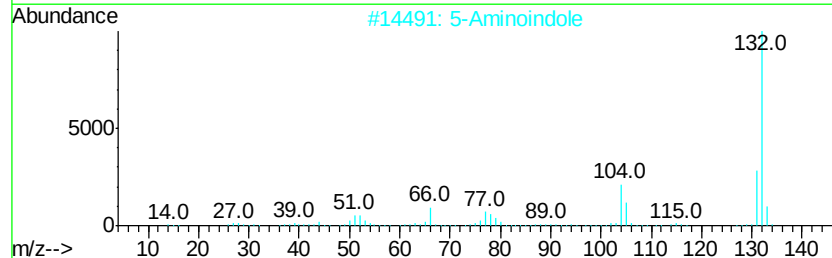
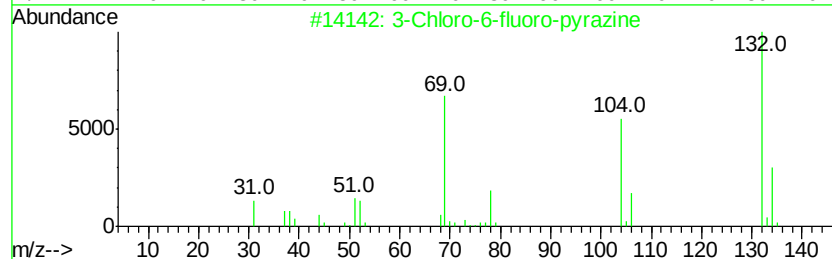
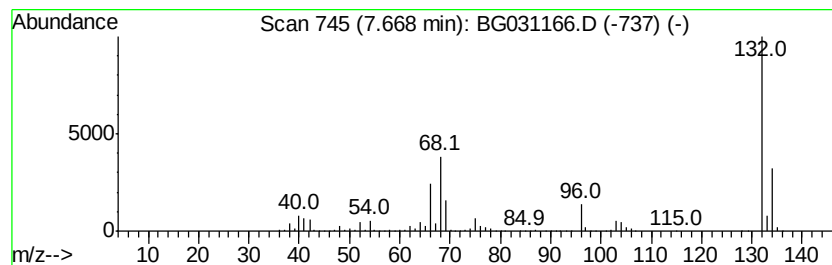
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Peak Number 1 unknown7.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.67	92.89 ng	1651770	1,4-Dichlorobenzene-d4	8.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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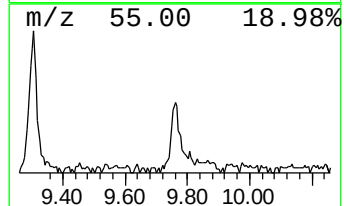
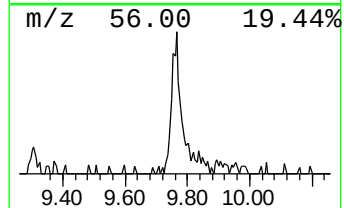
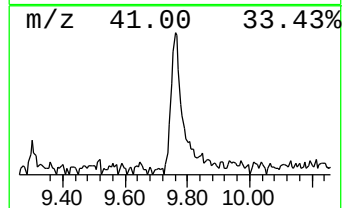
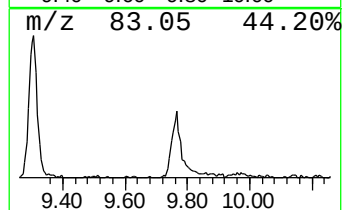
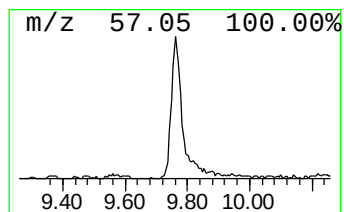
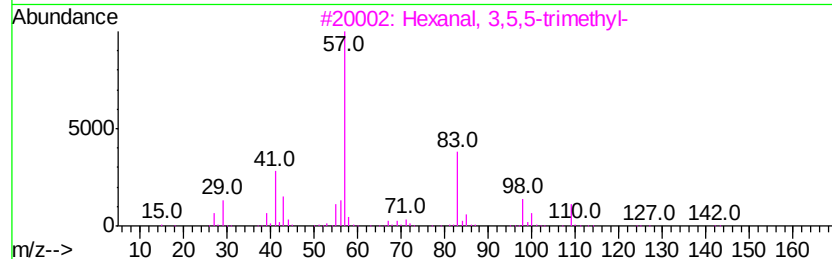
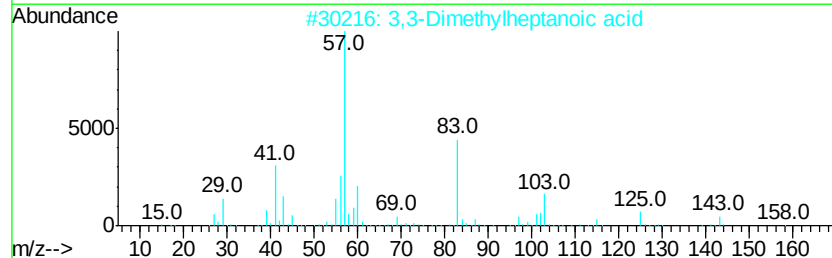
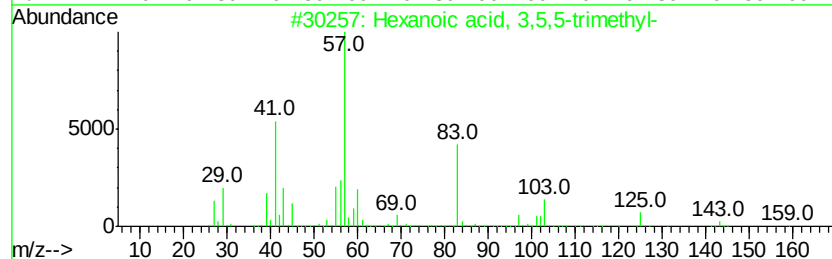
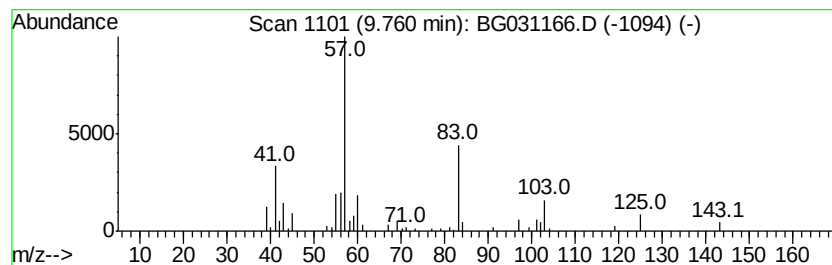
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Peak Number 3 Hexanoic acid, 3,5,5-trimet... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.76	4.20 ng	110952	Naphthalene-d8	10.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	90
2		3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	90
3		Hexanal, 3,5,5-trimethyl-	142	C9H18O	005435-64-3	38
4		4,4-Dimethyl-2-pentanol, chlorod...	228	C9H15ClF2O2	1000376-27-0	32
5		Propanoic acid, 2,2-dimethyl-, b...	158	C9H18O2	005129-37-3	27



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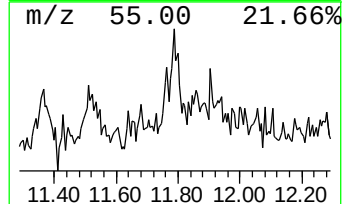
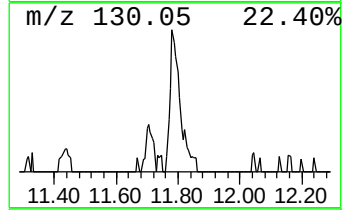
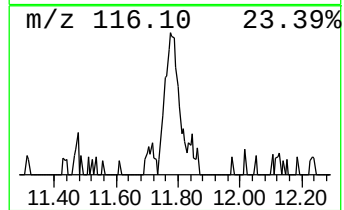
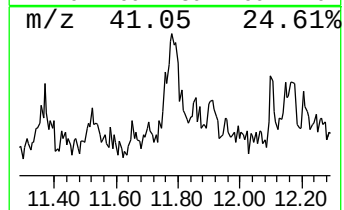
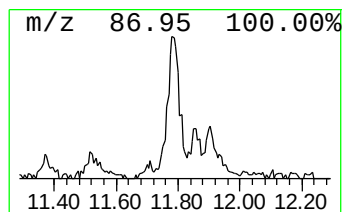
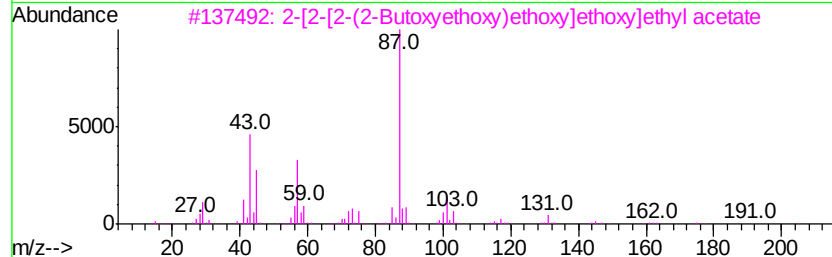
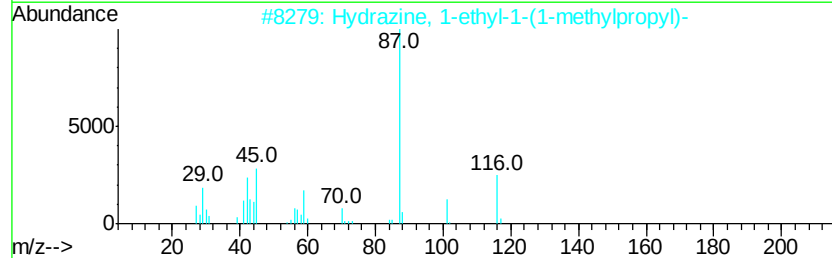
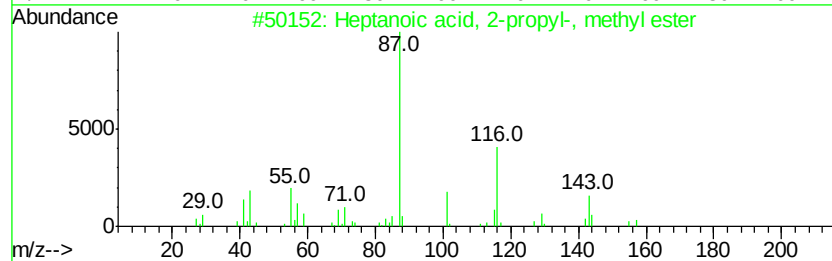
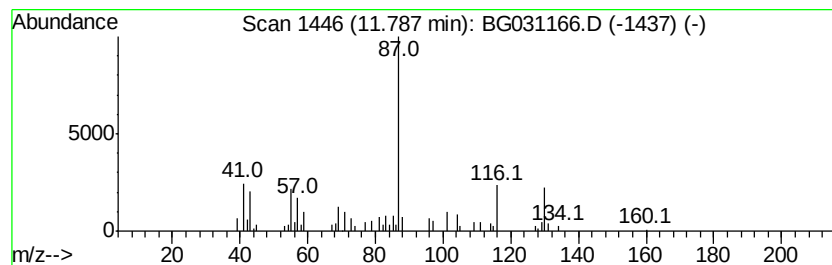
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Peak Number 4 Heptanoic acid, 2-propyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	2.81 ng	74282	Naphthalene-d8	10.95

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptanoic acid, 2-propyl-, methy...	186	C11H22O2	056247-53-1	59
2		Hydrazine, 1-ethyl-1-(1-methylpr...	116	C6H16N2	020325-97-7	53
3		2-[2-[2-(2-Butoxyethoxy)ethoxy]le...	292	C14H28O6	1000351-93-9	47
4		Hydrazine, 1,1-dipropyl-	116	C6H16N2	004986-50-9	47
5		Uridine, 2'-O-methyl-	258	C10H14N2O6	002140-76-3	47



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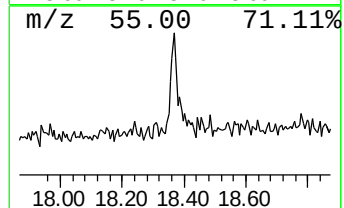
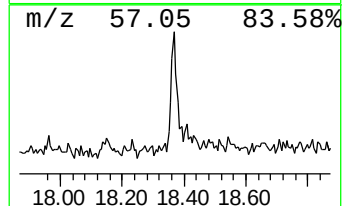
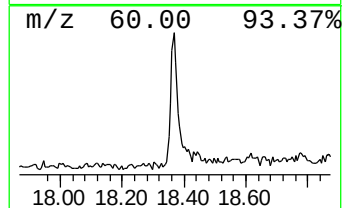
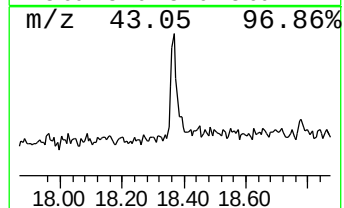
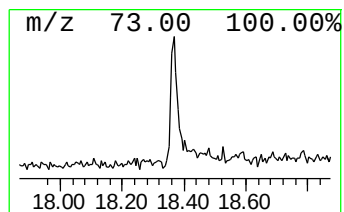
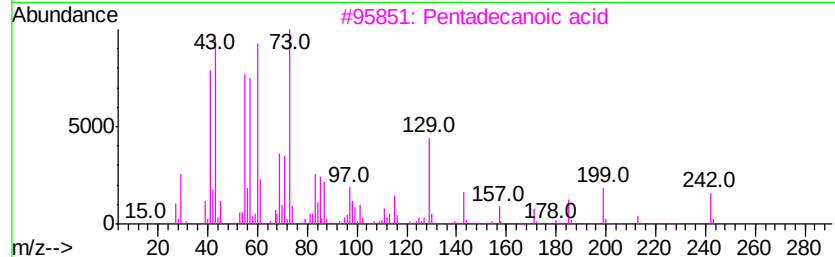
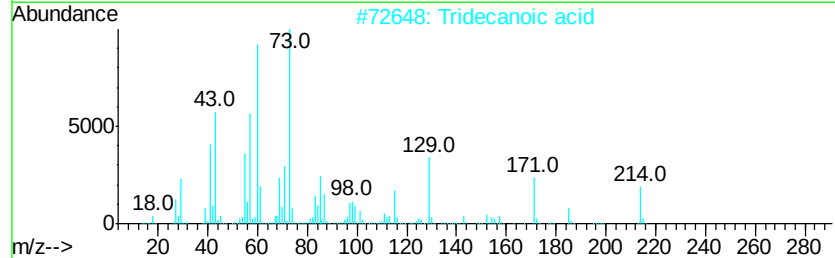
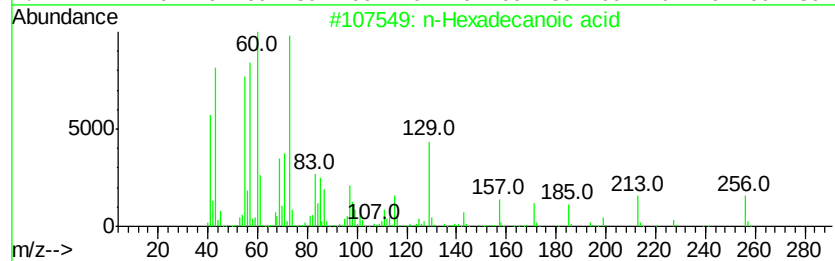
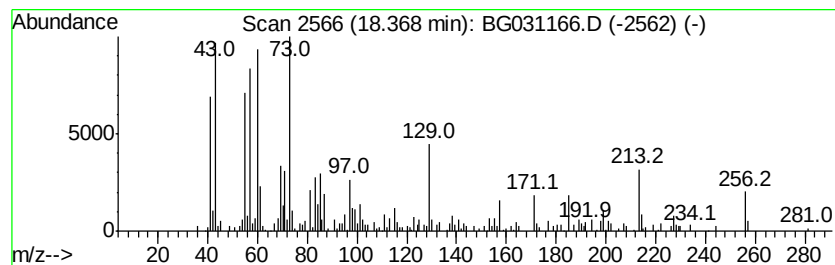
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.37	2.50 ng	128815	Phenanthrene-d10	17.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4		n-Decanoic acid	172	C10H20O2	000334-48-5	64
5		Dodecanoic acid	200	C12H24O2	000143-07-7	58



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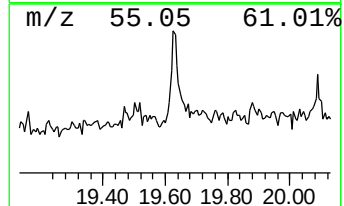
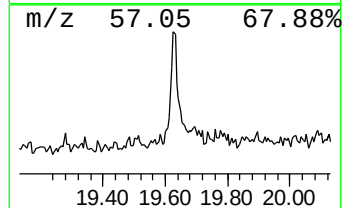
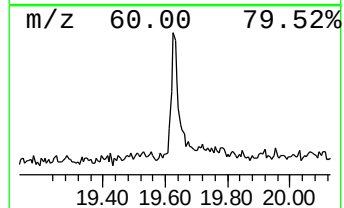
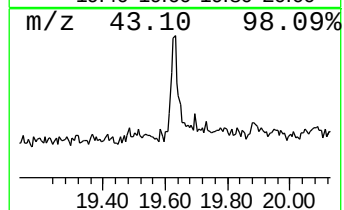
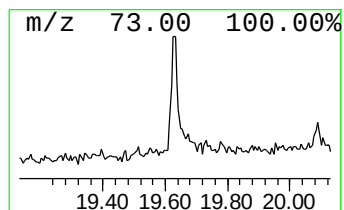
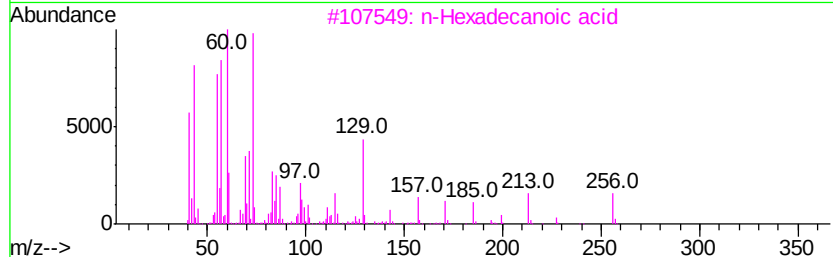
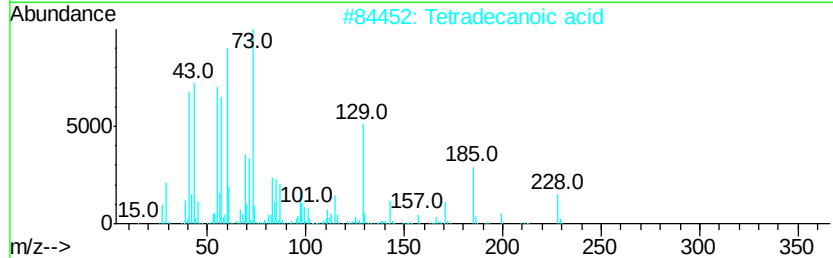
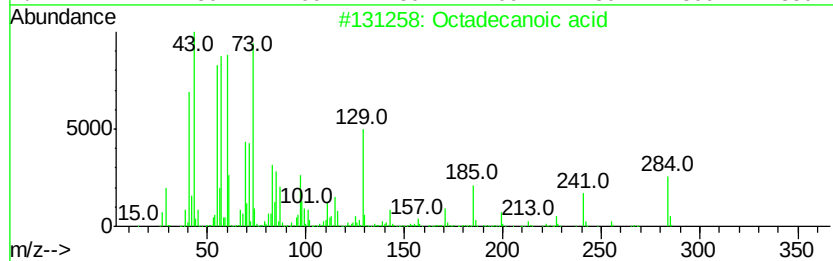
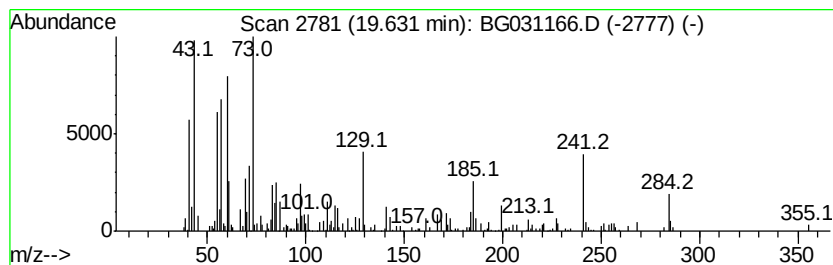
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Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.63	2.87 ng	147955	Phenanthrene-d10		17.50	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	95
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5		Dodecanoic acid	200	C12H24O2	000143-07-7	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown7.67	7.67	92.9	ng	1651770	1	8.14	355650	20.0
Hexanoic acid, 3,...	9.76	4.2	ng	110952	2	10.95	528796	20.0
Heptanoic acid, 2...	11.79	2.8	ng	74282	2	10.95	528796	20.0
n-Hexadecanoic acid	18.37	2.5	ng	128815	4	17.50	1029820	20.0
Octadecanoic acid	19.63	2.9	ng	147955	4	17.50	1029820	20.0