

Data Path : Z:\HPCHEM1\BNA G\DATA\BG112117\
 Data File : BG031165.D
 Acq On : 21 Nov 2017 22:58
 Operator : SJ/JU
 Sample : I6505-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 LW-03

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	5.697	403	410	421	rBV	483678	837712	15.35%	3.631%
2	7.301	674	683	700	rBV	296051	577006	10.57%	2.501%
3	7.671	737	746	758	rBV	935891	1659625	30.41%	7.194%
4	8.136	818	825	832	rBV	205115	351728	6.44%	1.525%
5	8.459	873	880	894	rBV	821082	1515574	27.77%	6.570%
6	9.305	1016	1024	1041	rBV	651848	1241522	22.75%	5.382%
7	9.763	1096	1102	1110	rBV	50453	107725	1.97%	0.467%
8	10.950	1296	1304	1320	rBV	273418	548376	10.05%	2.377%
9	11.790	1437	1447	1453	rBV5	22801	66754	1.22%	0.289%
10	13.382	1710	1718	1727	rBV	2060737	3275341	60.01%	14.199%
11	14.757	1942	1952	1959	rBV2	487049	827946	15.17%	3.589%
12	16.244	2198	2205	2215	rBV	1696347	2612810	47.87%	11.327%
13	17.495	2412	2418	2426	rBV2	650528	1025968	18.80%	4.448%
14	18.365	2562	2566	2576	rBV3	95780	172107	3.15%	0.746%
15	19.628	2777	2781	2790	rBV2	125169	209406	3.84%	0.908%
16	20.086	2854	2859	2866	rVB	3908098	5458016	100.00%	23.661%
17	21.767	3139	3145	3154	rVB	788632	1310961	24.02%	5.683%
18	25.075	3698	3708	3720	rVB2	429505	1269447	23.26%	5.503%

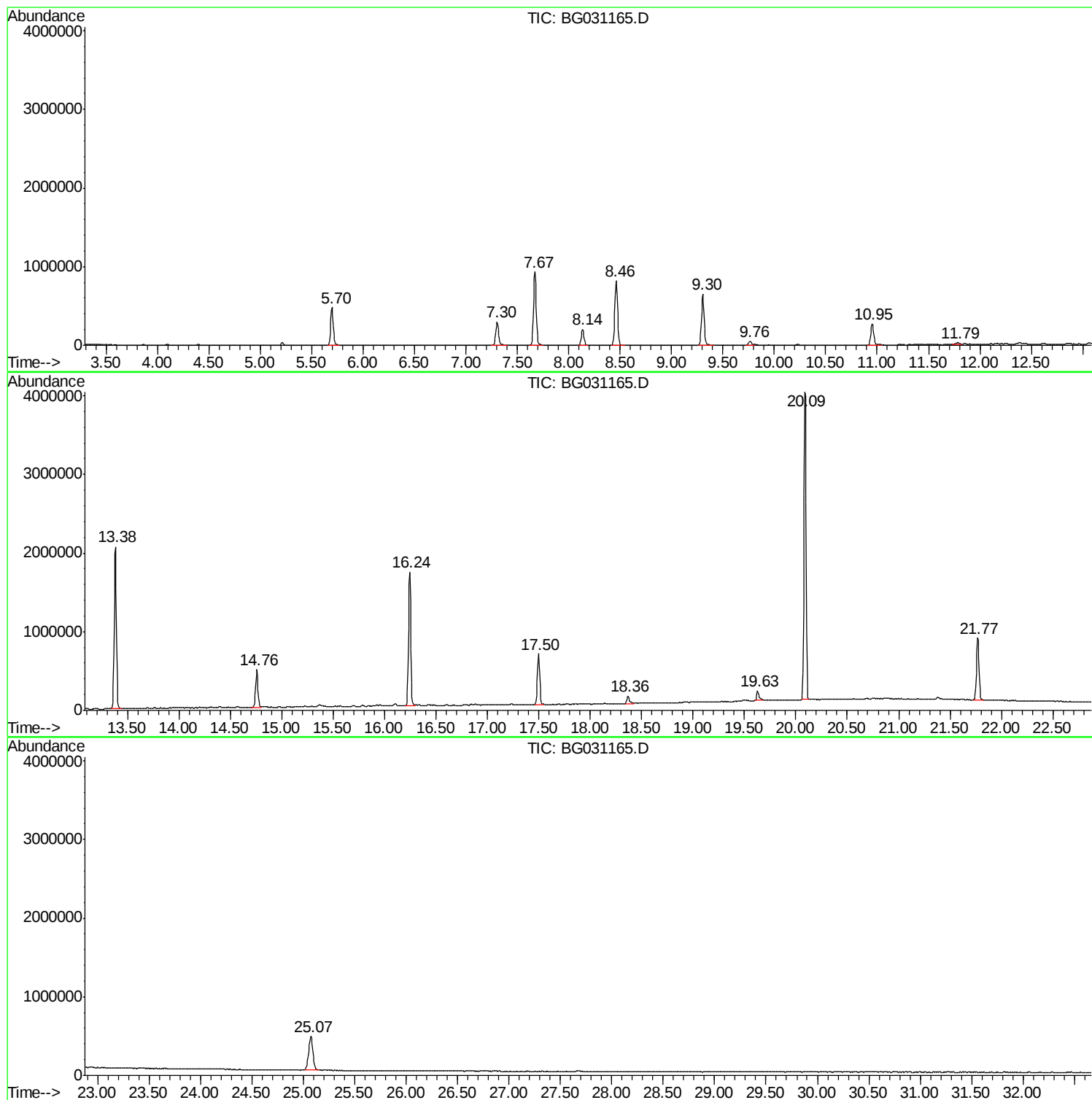
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG111017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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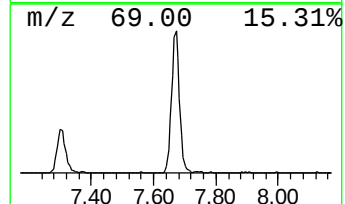
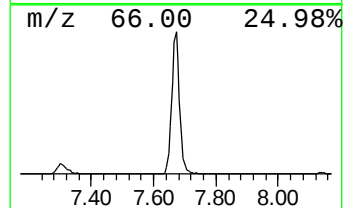
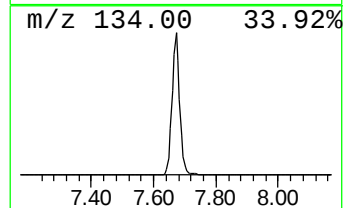
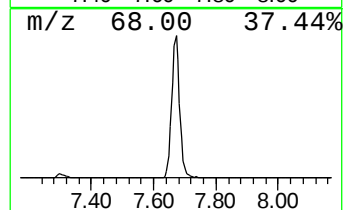
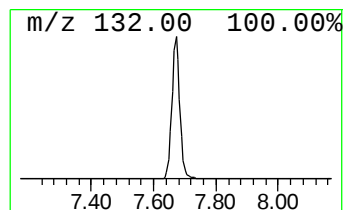
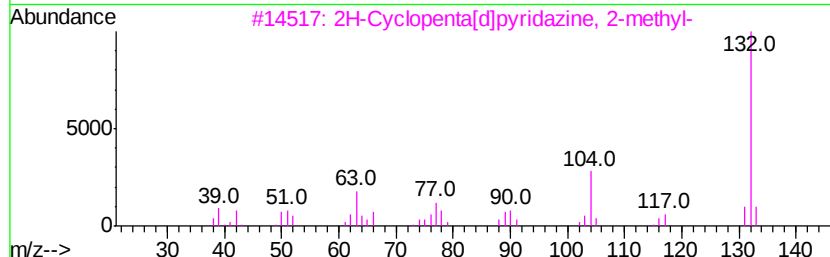
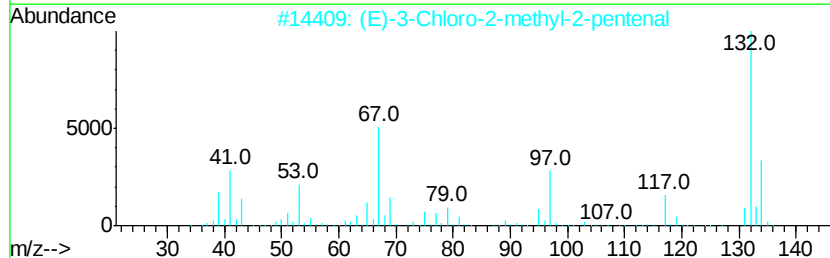
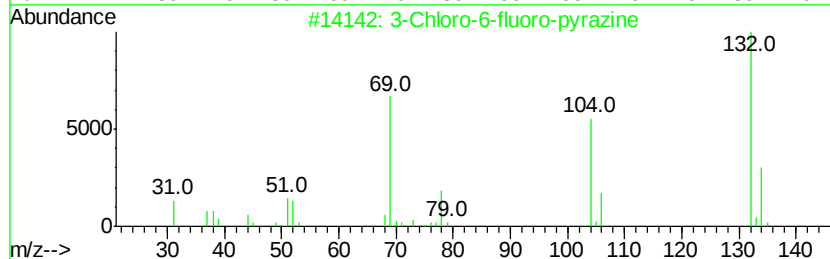
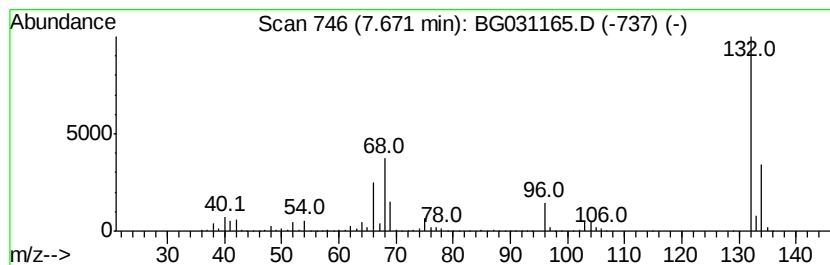
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TIC Library : C:\Database\NIST11.L
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Peak Number 1 unknown7.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.67	94.37 ng	1659630	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	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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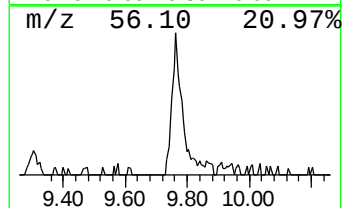
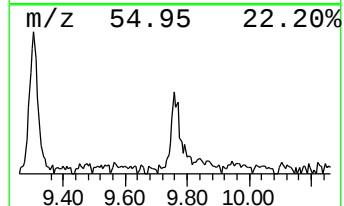
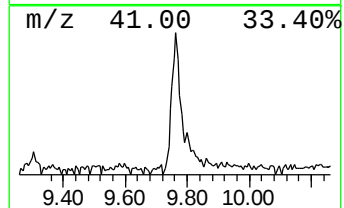
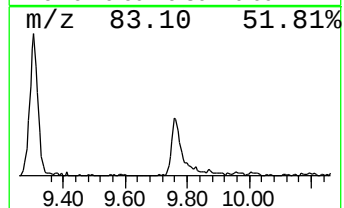
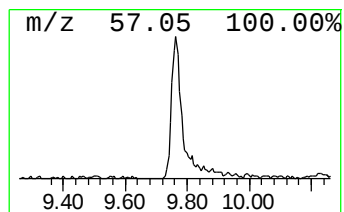
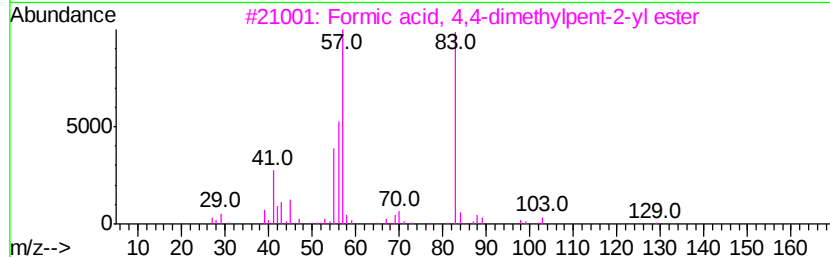
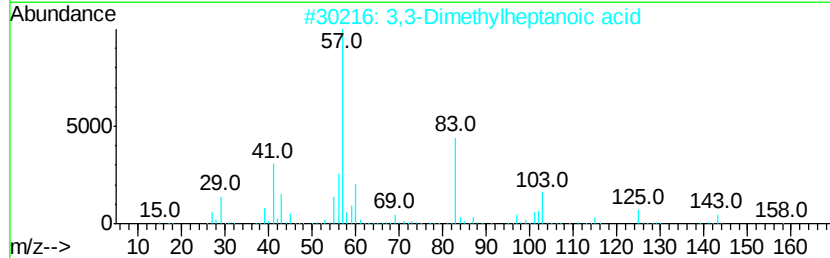
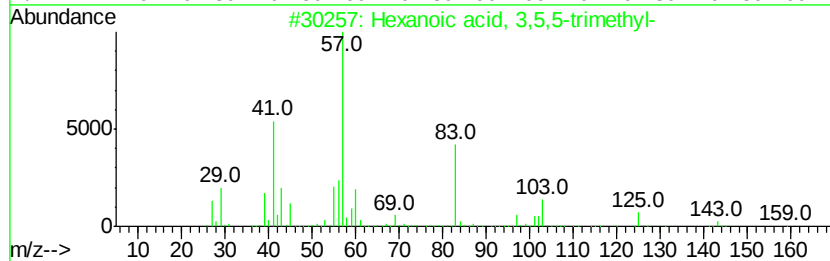
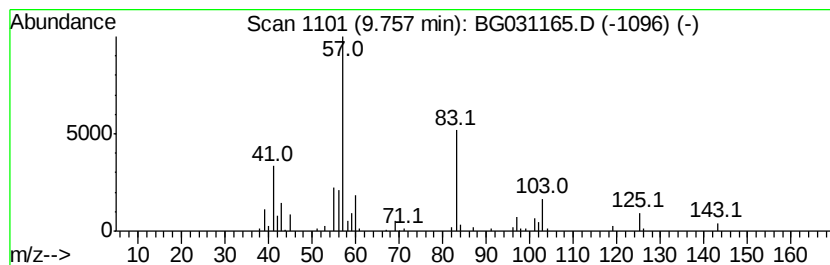
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Peak Number 3 Hexanoic acid, 3,5,5-trimet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.76	3.93 ng	107725	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	83
3		Formic acid, 4,4-dimethylpent-2-...	144	C8H16O2	1000368-69-9	38
4		4,4-Dimethyl-2-pentanol, chlorod...	228	C9H15ClF2O2	1000376-27-0	37
5		2-(2-Butoxyethoxy)acetic acid	176	C8H16O4	082941-26-2	32



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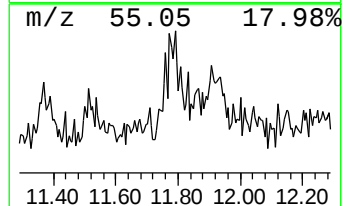
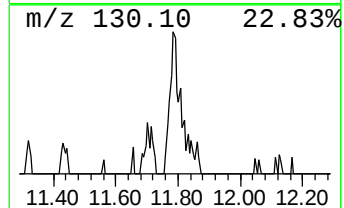
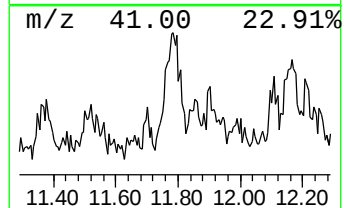
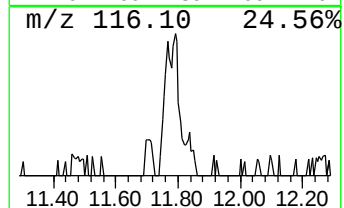
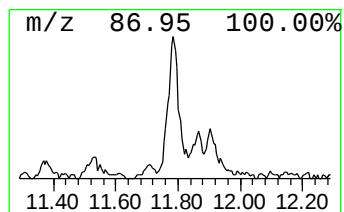
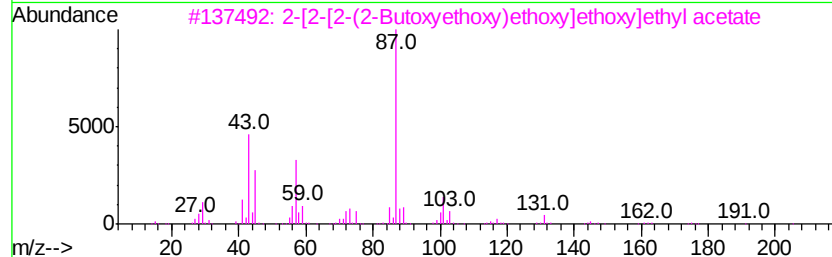
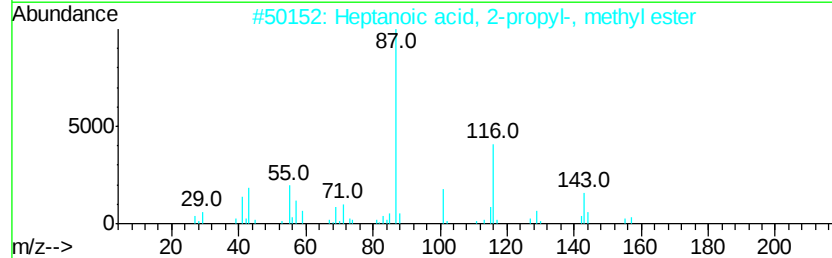
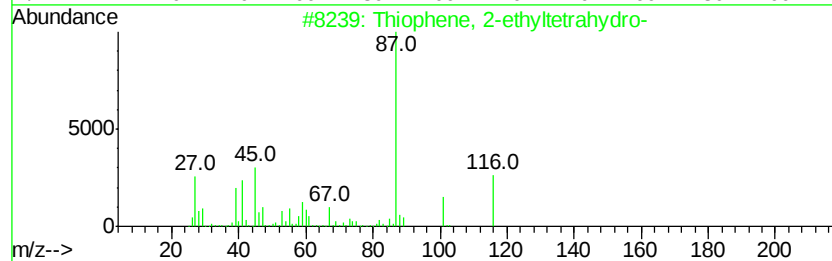
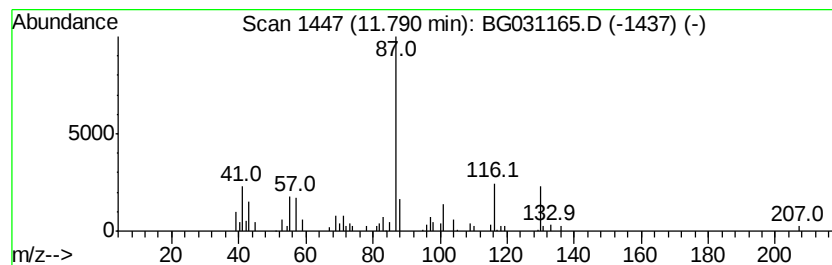
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Peak Number 4 Thiophene, 2-ethyltetrahydro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	2.43 ng	66754	Naphthalene-d8	10.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	53
2		Heptanoic acid, 2-propyl-, methyl...	186	C11H22O2	056247-53-1	53
3		2-[2-[2-(2-Butoxyethoxy)ethoxy]ethyl...	292	C14H28O6	1000351-93-9	47
4		.alpha.-D-Xylofuranoside, methyl...	192	C8H16O5	035007-52-4	47
5		1,3-Dioxolane-2-propanol, 2-meth...	188	C9H16O4	029021-95-2	43



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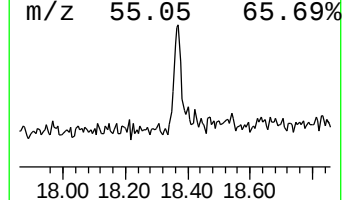
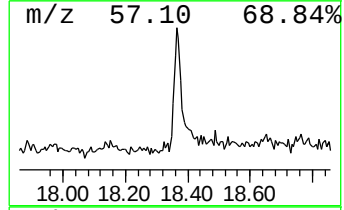
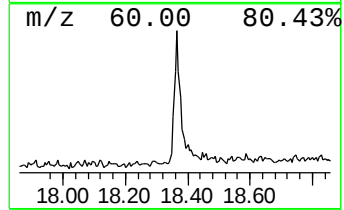
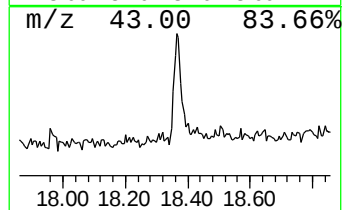
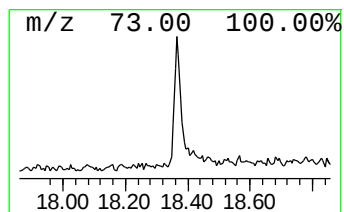
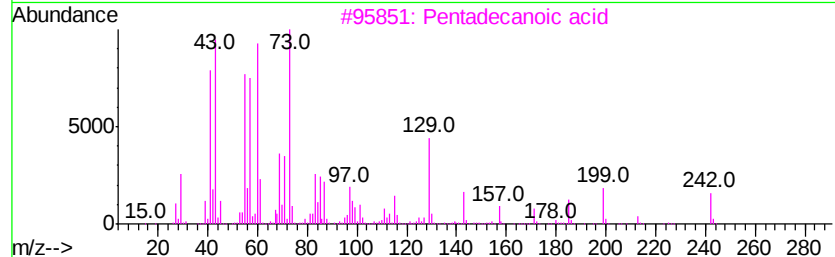
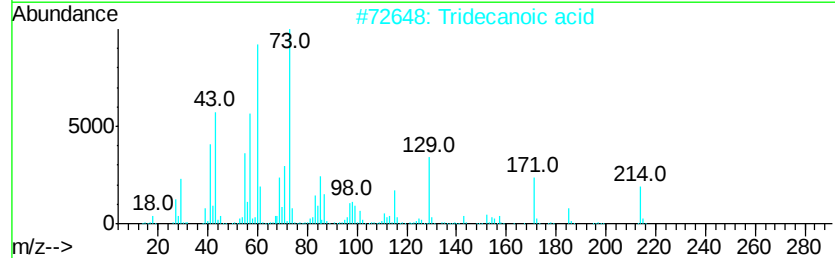
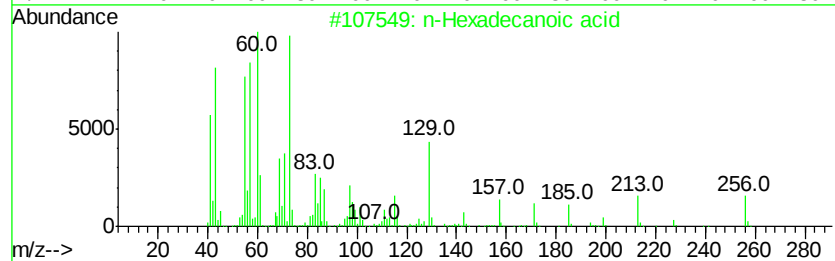
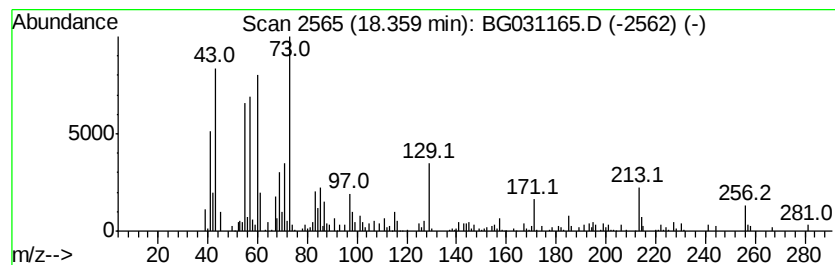
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	3.36 ng	172107	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	89
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4		Dodecanoic acid	200	C12H24O2	000143-07-7	64
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	59



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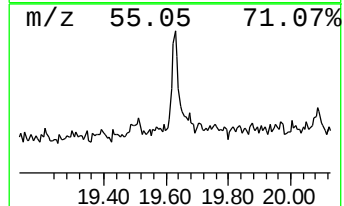
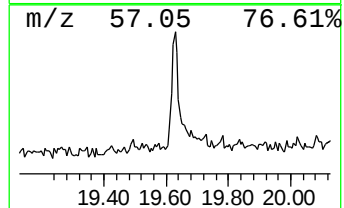
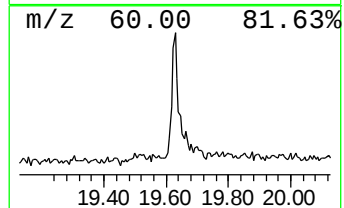
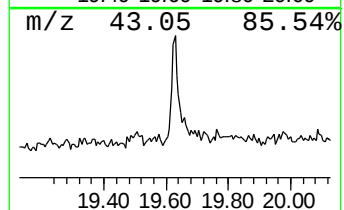
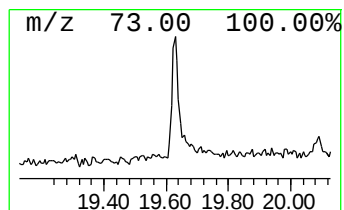
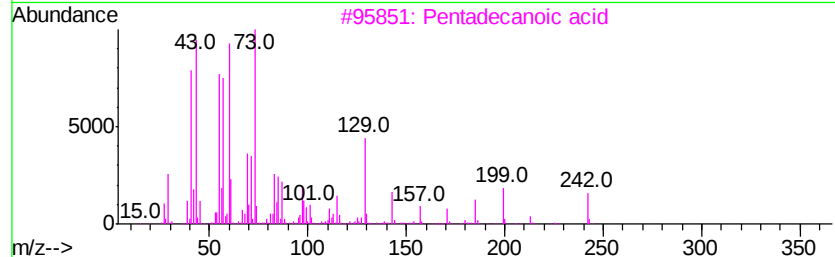
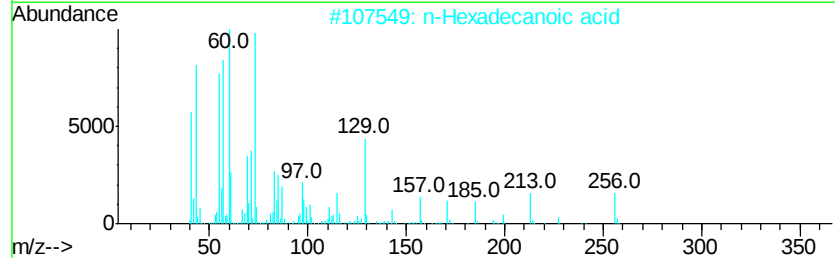
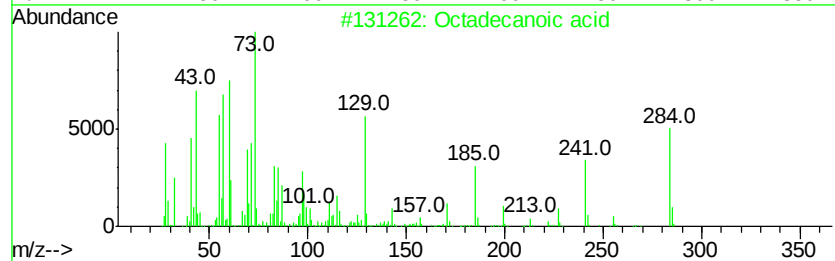
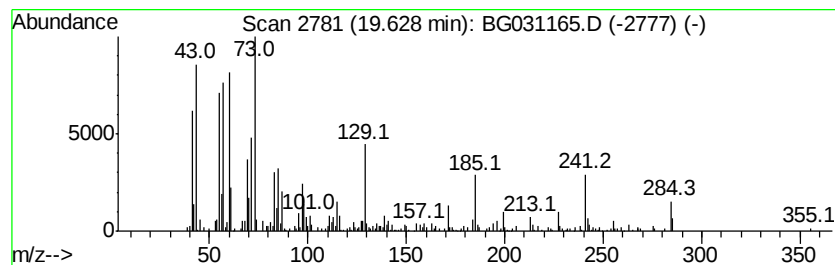
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Peak Number 6 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.63	4.08 ng	209406	Phenanthrene-d10	17.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	93
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5		Octadecanoic acid, 2-(2-hydroxy...	372	C22H44O4	000106-11-6	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown7.67	7.67	94.4	ng	1659630	1	8.14	351728	20.0
Hexanoic acid, 3,...	9.76	3.9	ng	107725	2	10.95	548376	20.0
Thiophene, 2-ethy...	11.79	2.4	ng	66754	2	10.95	548376	20.0
n-Hexadecanoic acid	18.36	3.4	ng	172107	4	17.50	1025970	20.0
Octadecanoic acid	19.63	4.1	ng	209406	4	17.50	1025970	20.0