

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080615\
 Data File : BF080901.D
 Acq On : 6 Aug 2015 21:34
 Operator : TP/UM
 Sample : G3196-02
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DUP

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_F\METHODS\8270-BF080615.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	4.281	191	192	196	rBV2	15554	24170	1.39%	0.203%
2	4.956	249	251	254	rBV	376776	396383	22.84%	3.332%
3	5.390	286	289	291	rBV	474375	602325	34.71%	5.063%
4	5.802	324	325	328	rBV	17956	19317	1.11%	0.162%
5	6.430	378	380	382	rBV	528714	469178	27.03%	3.944%
6	6.567	389	392	394	rBV	1077312	906881	52.25%	7.623%
7	6.807	411	413	415	rBV	441440	371910	21.43%	3.126%
8	6.967	424	427	429	rVB	690353	864940	49.84%	7.270%
9	7.367	459	462	465	rBV	788953	718034	41.37%	6.035%
10	8.087	523	525	528	rBV	424334	453988	26.16%	3.816%
11	9.173	617	620	622	rBV	1660093	1606491	92.56%	13.503%
12	9.562	652	654	656	rBV	185839	143619	8.28%	1.207%
13	9.848	676	679	681	rBV	483091	544811	31.39%	4.579%
14	10.259	711	715	716	rBV	18776	22426	1.29%	0.188%
15	10.282	716	717	719	rVB	24387	18352	1.06%	0.154%
16	10.625	745	747	750	rBV2	839532	910998	52.49%	7.657%
17	10.751	756	758	762	rBV	32851	44286	2.55%	0.372%
18	11.196	795	797	799	rBV	33269	40823	2.35%	0.343%
19	11.322	806	808	810	rBV	707506	593089	34.17%	4.985%
20	11.631	832	835	837	rBV	50075	76227	4.39%	0.641%
21	11.859	853	855	857	rBV	73165	69954	4.03%	0.588%
22	12.031	868	870	872	rBV	23745	19224	1.11%	0.162%
23	12.111	875	877	879	rVB	99108	79406	4.58%	0.667%
24	12.511	906	912	915	rBV4	7786	31884	1.84%	0.268%
25	12.911	944	947	949	rBV	1826493	1735547	100.00%	14.588%
26	13.951	1035	1038	1040	rVB	667177	606308	34.93%	5.096%
27	15.357	1158	1161	1164	rBV	459441	526561	30.34%	4.426%

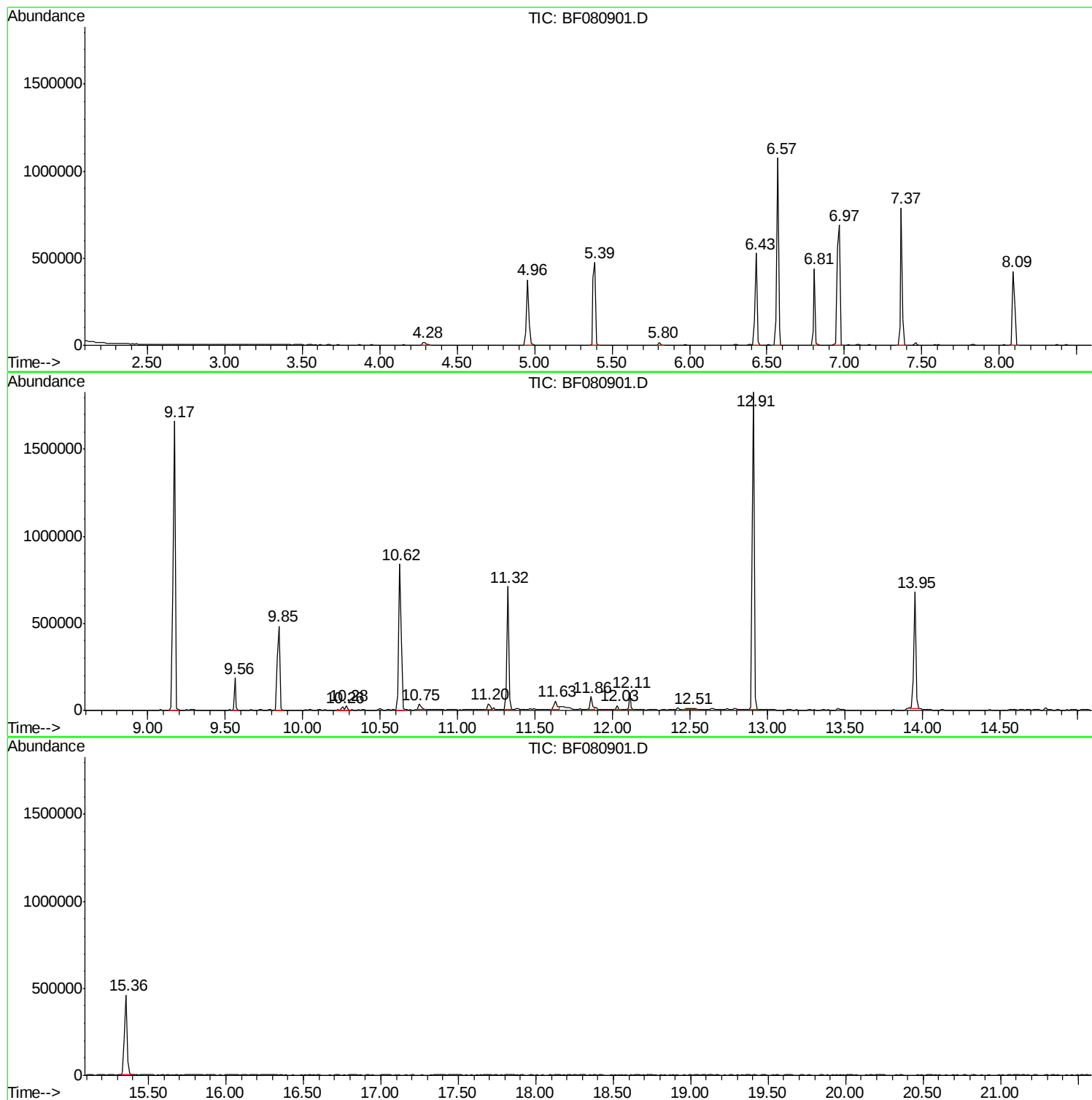
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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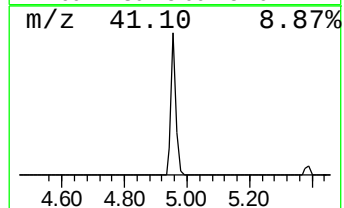
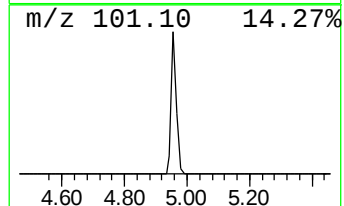
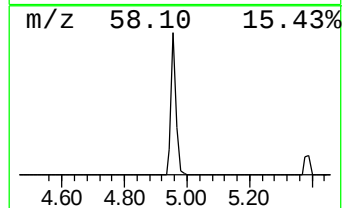
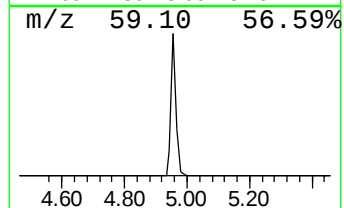
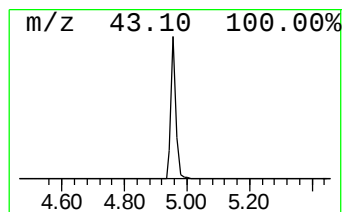
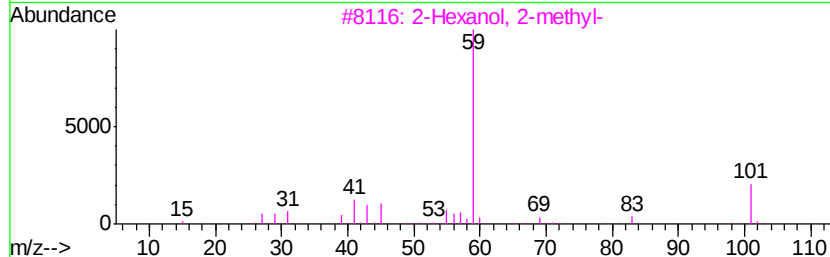
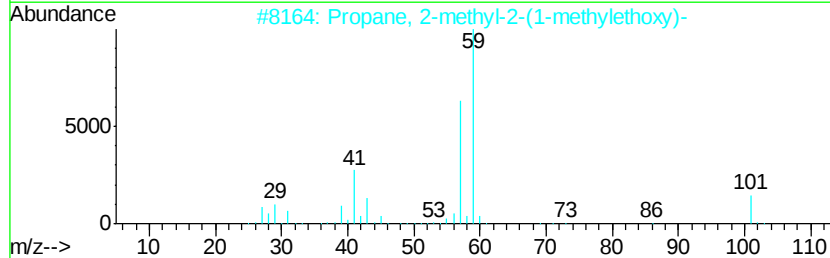
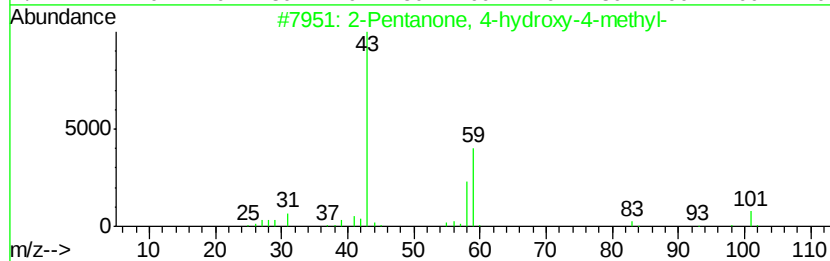
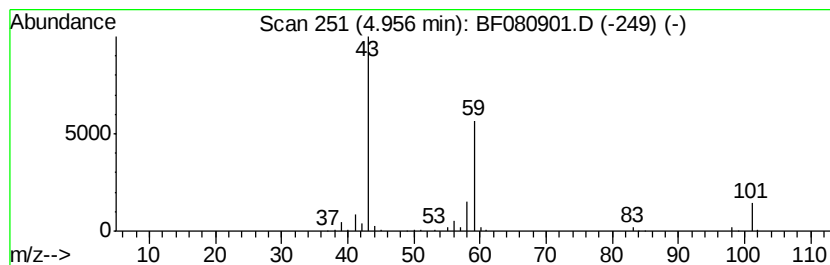
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	21.32 ng	396383	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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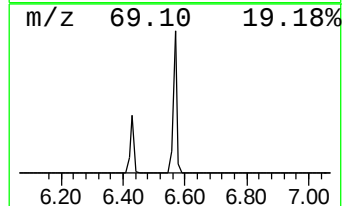
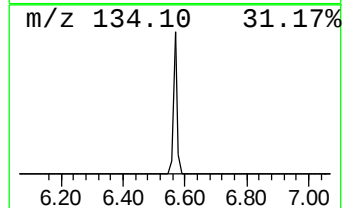
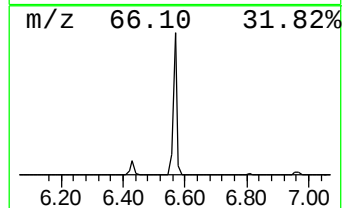
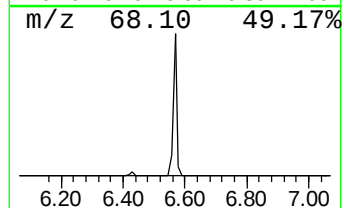
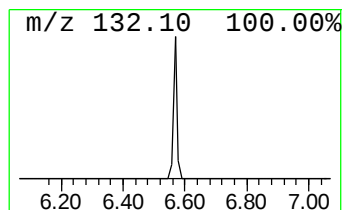
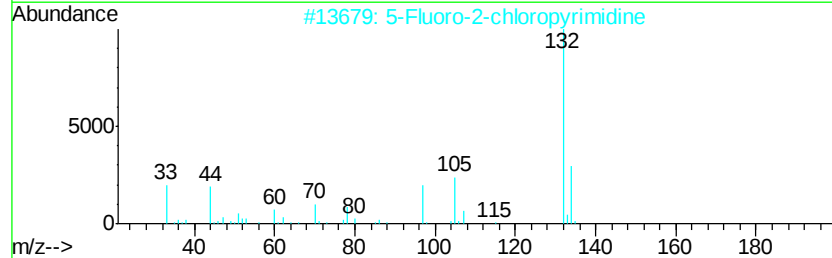
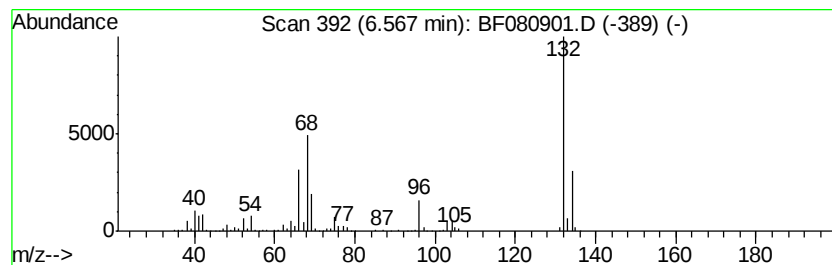
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080615.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	48.77 ng	906881	1,4-Dichlorobenzene-d4	6.81

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



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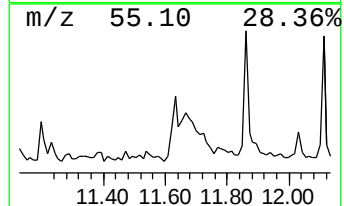
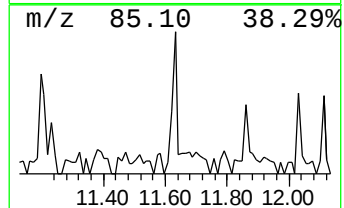
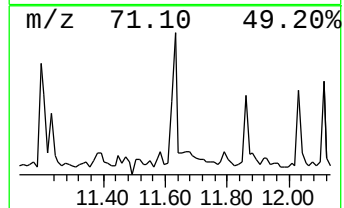
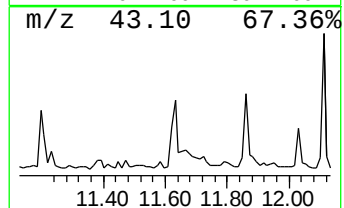
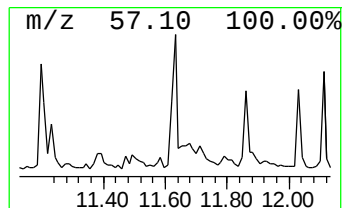
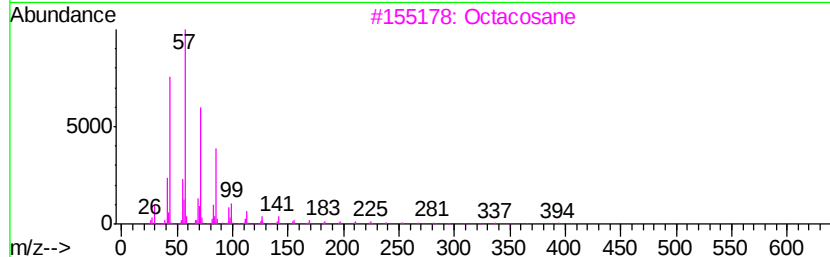
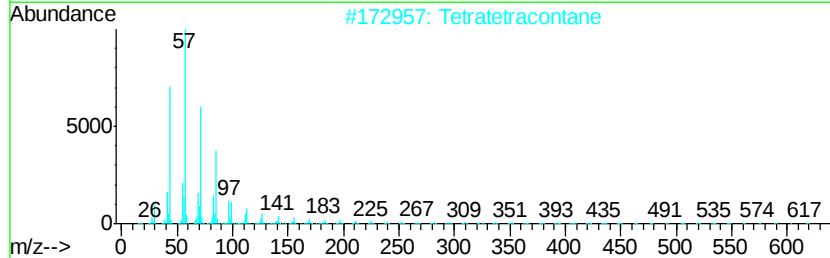
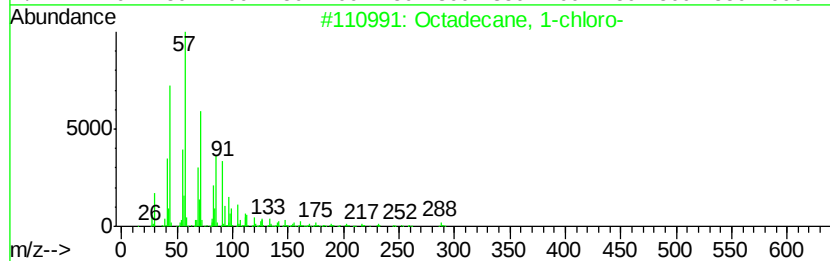
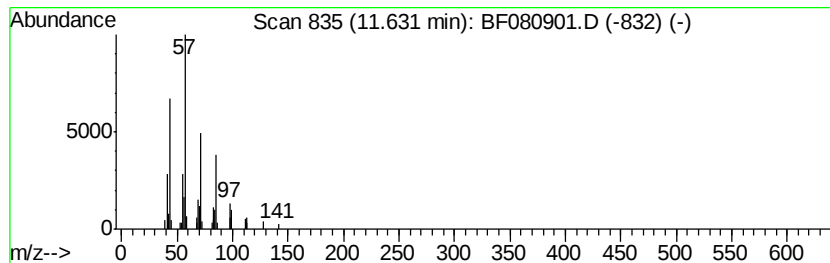
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Peak Number 4 Octadecane, 1-chloro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.63	2.57 ng	76227	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	90
2		Tetratetracontane	619	C44H90	007098-22-8	90
3		Octacosane	394	C28H58	000630-02-4	87
4		Tridecane	184	C13H28	000629-50-5	86
5		Pentadecane	212	C15H32	000629-62-9	86



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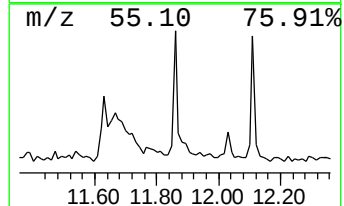
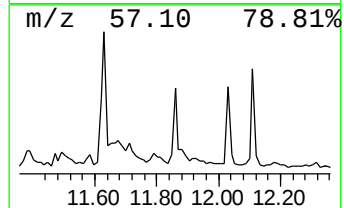
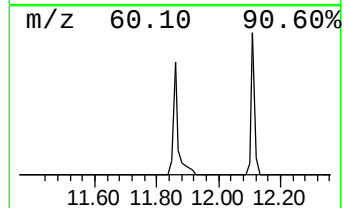
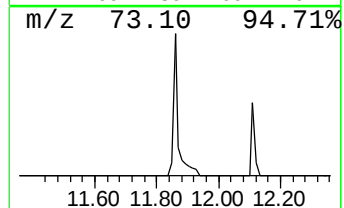
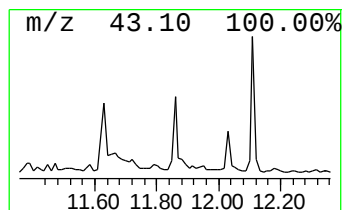
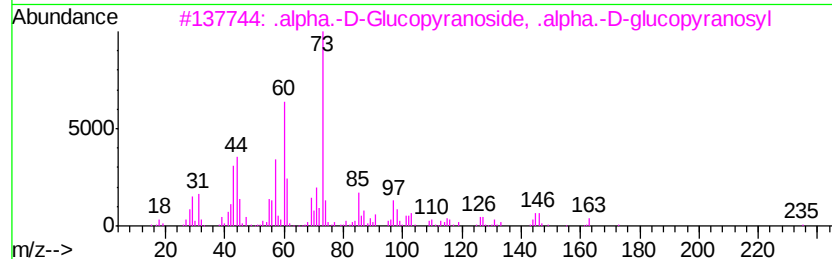
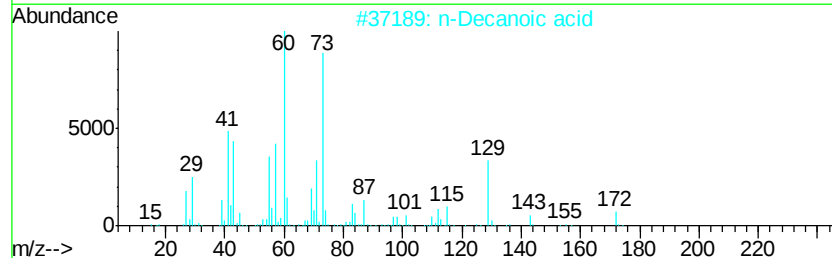
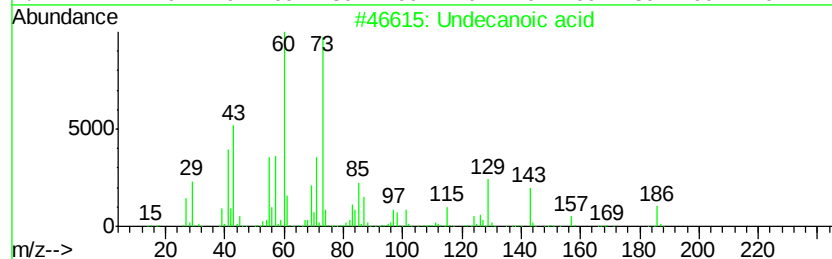
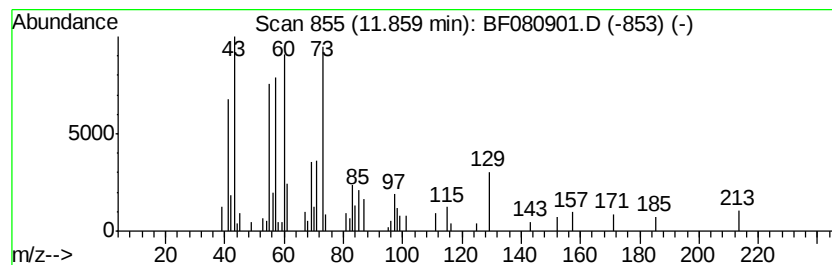
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Peak Number 5 Undecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.86	2.36 ng	69954	Phenanthrene-d10		11.32
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	72
2	n-Decanoic acid	172	C10H20O2	000334-48-5	50
3	.alpha.-D-Glucopyranoside, .alph...	342	C12H22O11	000099-20-7	43
4	Methyl-.alpha.-d-ribofuranoside	164	C6H12O5	1000129-83-1	43
5	Heptanoic acid	130	C7H14O2	000111-14-8	35



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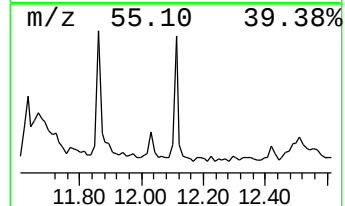
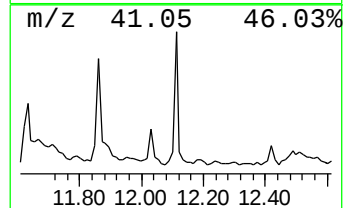
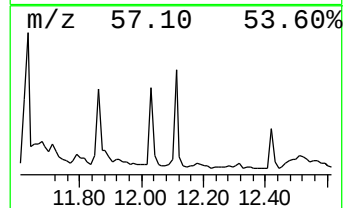
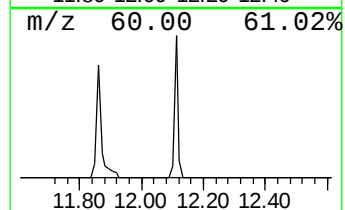
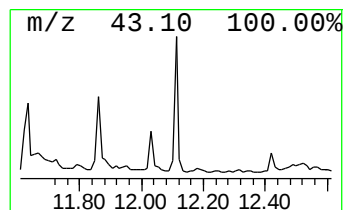
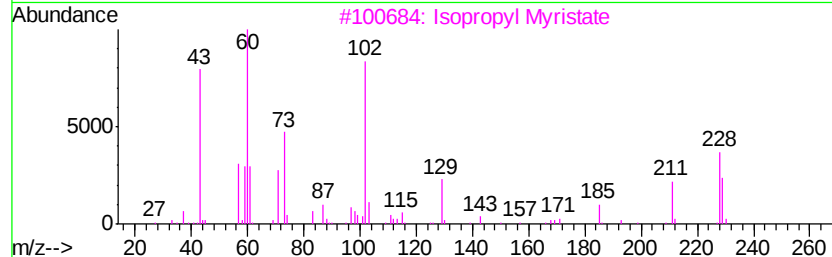
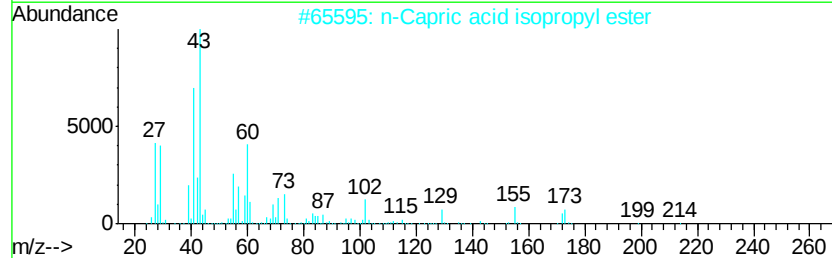
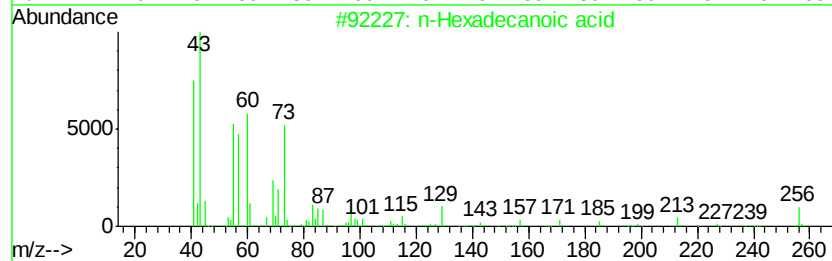
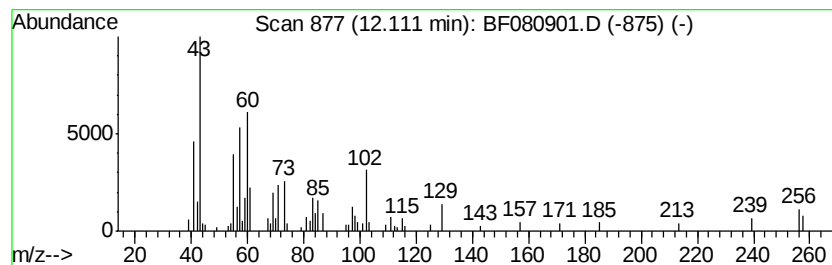
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.11	2.68 ng	79406	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
2		n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	53
3		Isopropyl Myristate	270	C17H34O2	000110-27-0	42
4		Nonanoic acid, 1-methylethyl ester	200	C12H24O2	028267-32-5	42
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.96	21.3	ng	396383	1	6.81	371910	20.0
unknown6.57	6.57	48.8	ng	906881	1	6.81	371910	20.0
Octadecane, 1-chl...	11.63	2.6	ng	76227	4	11.32	593089	20.0
Undecanoic acid	11.86	2.4	ng	69954	4	11.32	593089	20.0
n-Hexadecanoic acid	12.11	2.7	ng	79406	4	11.32	593089	20.0