

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090115\
 Data File : BF081323.D
 Acq On : 2 Sep 2015 1:15
 Operator : UM/IZ
 Sample : G3479-11
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COFF-3-6(0-2)

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_F\METHODS\8270-BF090115.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	4.456	246	251	262	rVB	566436	1195544	57.42%	7.113%
2	4.936	291	293	296	rBV	1312512	1787979	85.88%	10.637%
3	6.056	388	391	393	rBV	1748627	2081945	100.00%	12.386%
4	6.159	397	400	402	rBV	1436661	1848342	88.78%	10.996%
5	6.387	418	420	422	rBV	440246	368120	17.68%	2.190%
6	6.547	431	434	436	rBV	1080785	1313598	63.09%	7.815%
7	6.959	468	470	473	rBV	858930	1124658	54.02%	6.691%
8	7.679	530	533	535	rBV	476766	470545	22.60%	2.799%
9	8.765	625	628	630	rBV	1288004	1738452	83.50%	10.343%
10	9.165	660	663	665	rBV	385814	365698	17.57%	2.176%
11	9.416	683	685	687	rBV	571847	499523	23.99%	2.972%
12	10.194	751	753	756	rBV2	816963	978737	47.01%	5.823%
13	10.354	765	767	770	rBV	19379	25358	1.22%	0.151%
14	10.879	811	813	815	rBV	611780	510307	24.51%	3.036%
15	11.451	861	863	869	rBV2	50719	67094	3.22%	0.399%
16	12.468	949	952	954	rBV	1570712	1469189	70.57%	8.741%
17	13.394	1031	1033	1039	rBV	91173	195251	9.38%	1.162%
18	13.485	1039	1041	1044	rVV	451509	410406	19.71%	2.442%
19	14.800	1153	1156	1158	rBV	313289	317592	15.25%	1.889%
20	15.280	1193	1198	1204	rBV3	11500	40275	1.93%	0.240%

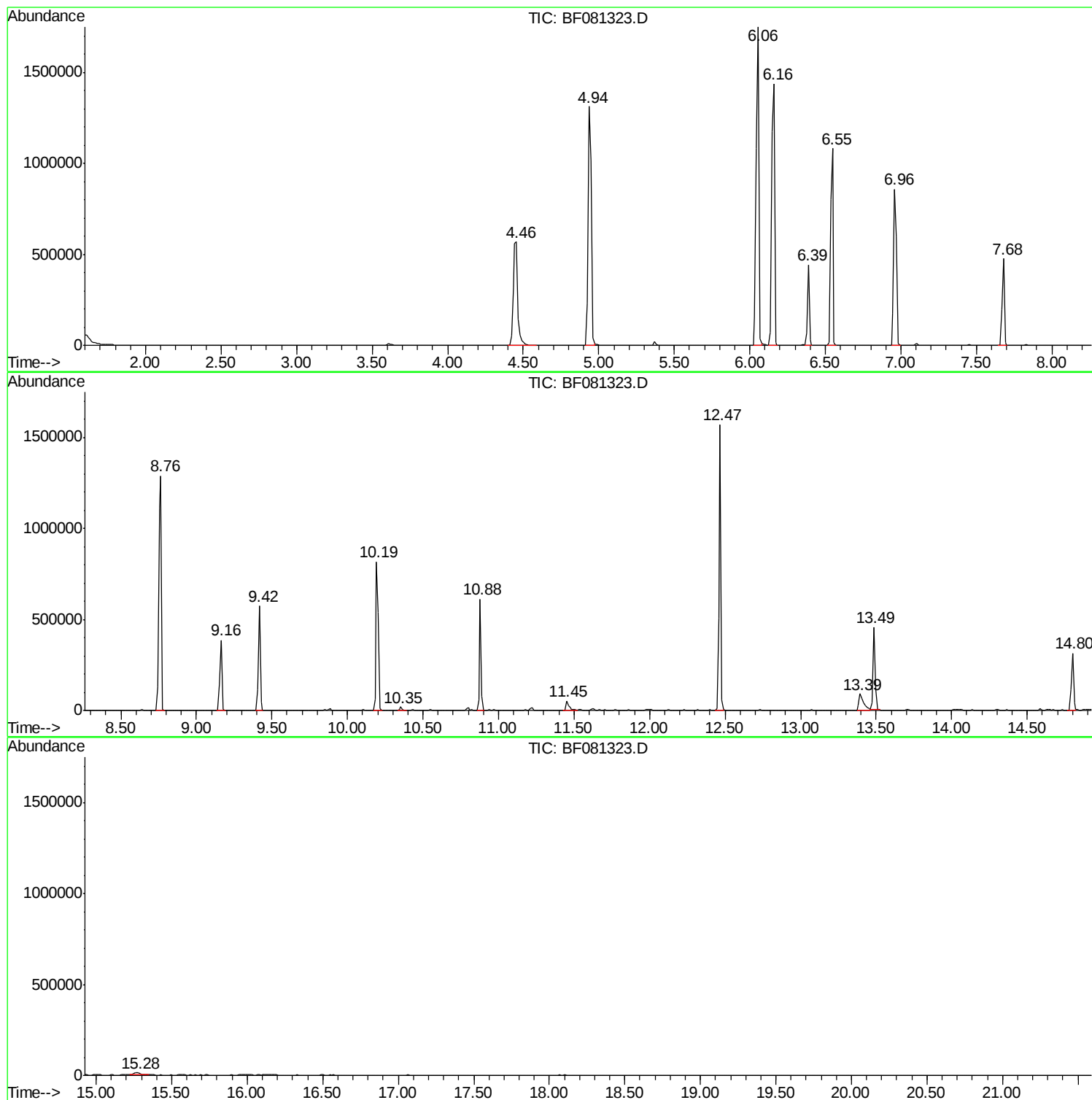
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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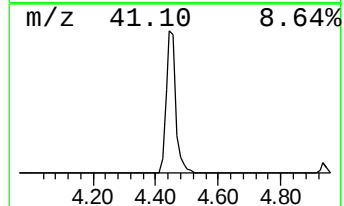
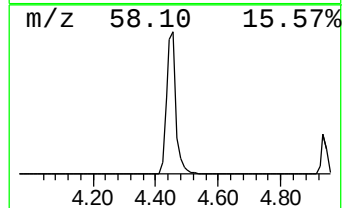
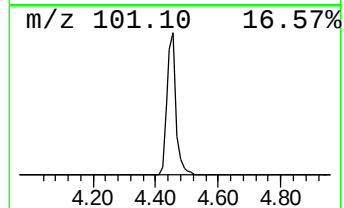
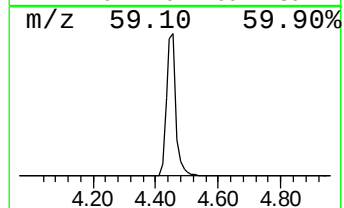
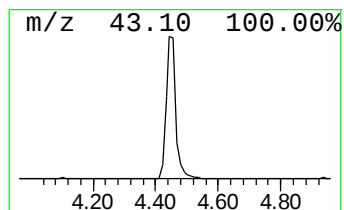
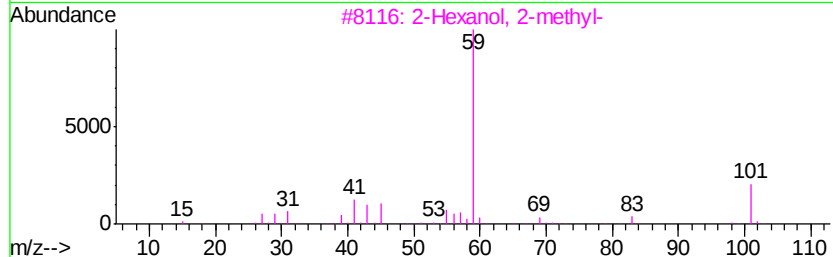
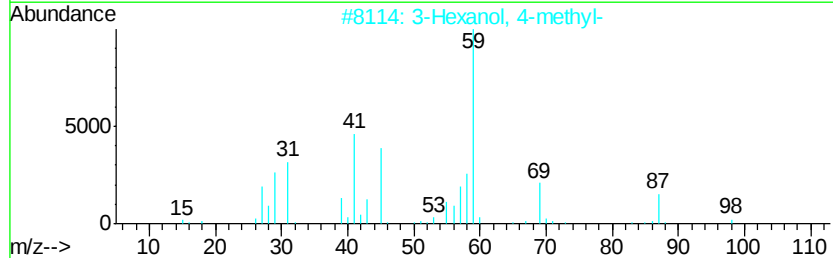
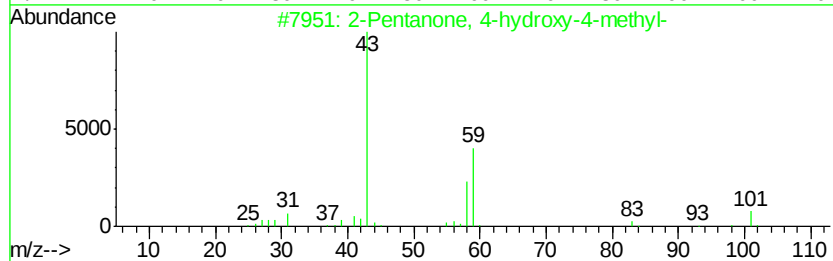
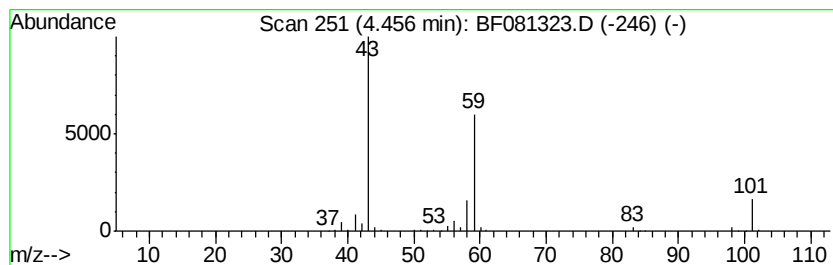
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.46	64.95 ng	1195540	1,4-Dichlorobenzene-d4	6.39

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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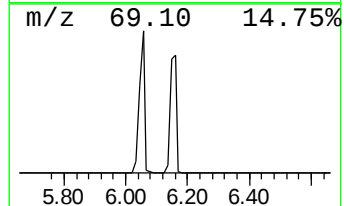
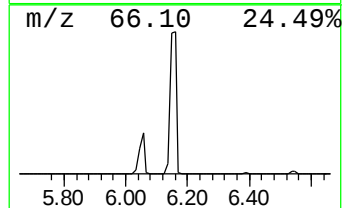
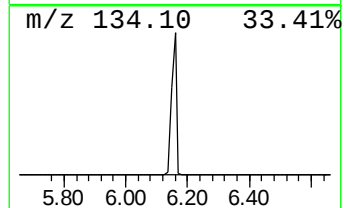
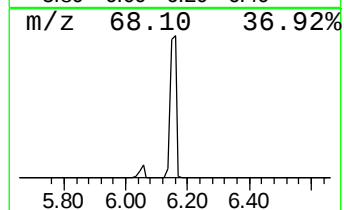
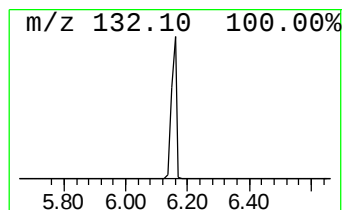
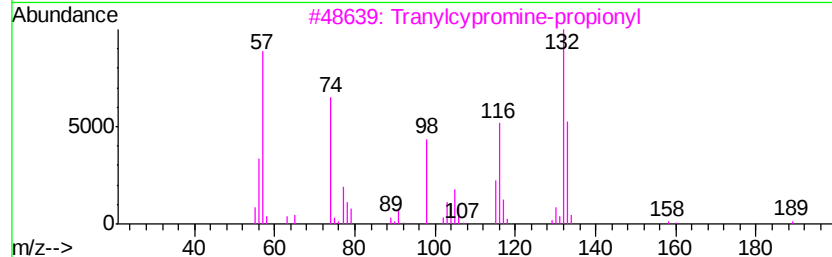
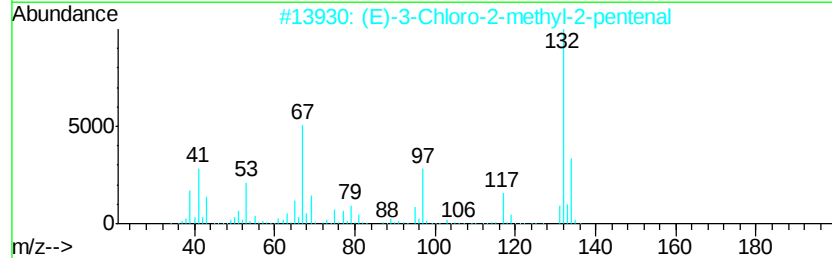
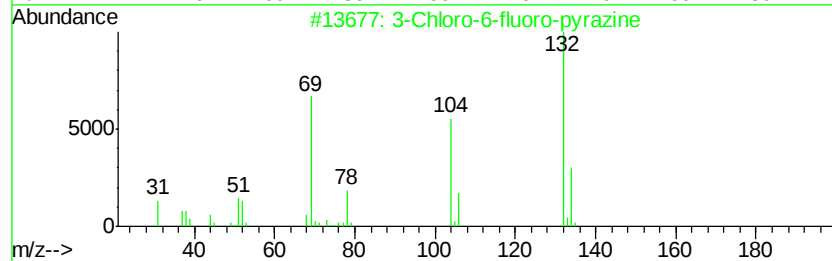
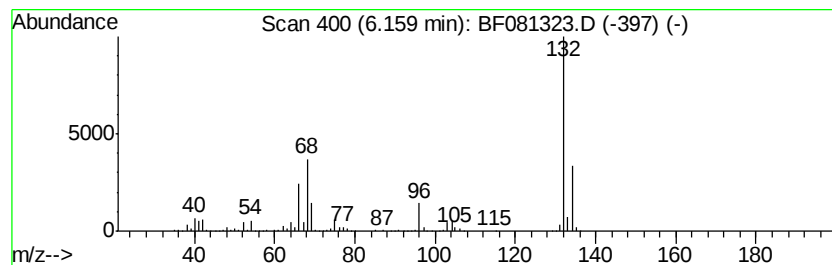
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Peak Number 2 unknown6.16 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.16	100.42 ng	1848340	1,4-Dichlorobenzene-d4	6.39

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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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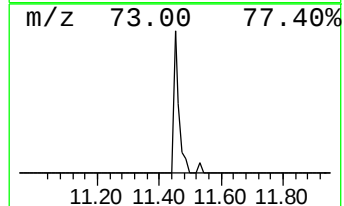
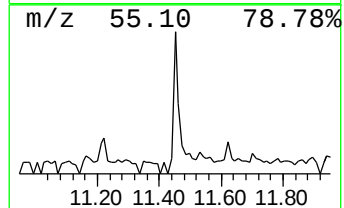
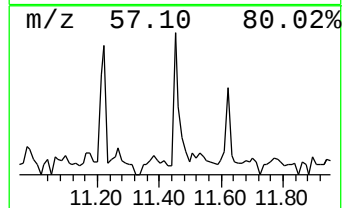
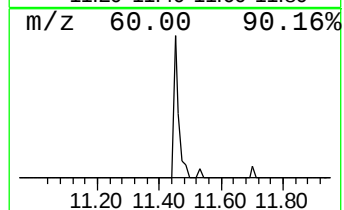
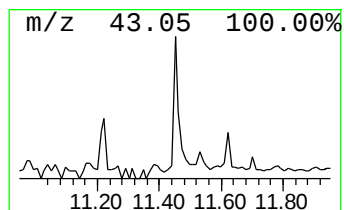
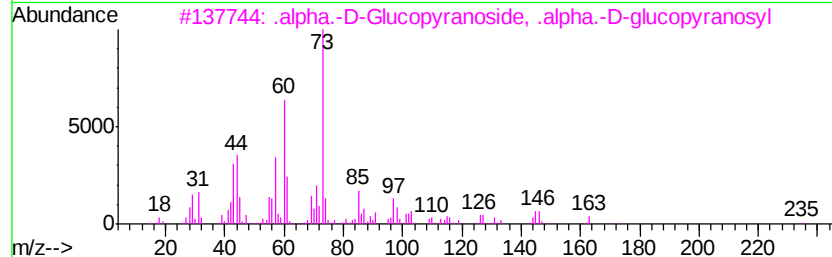
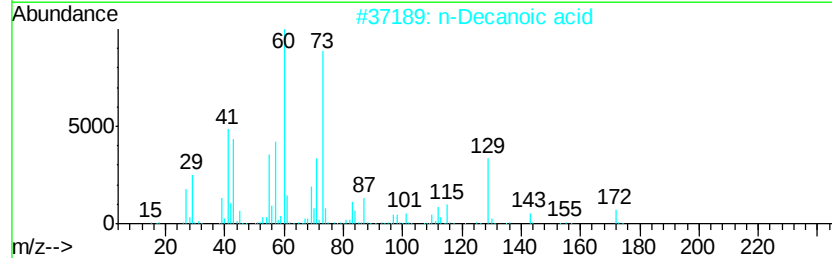
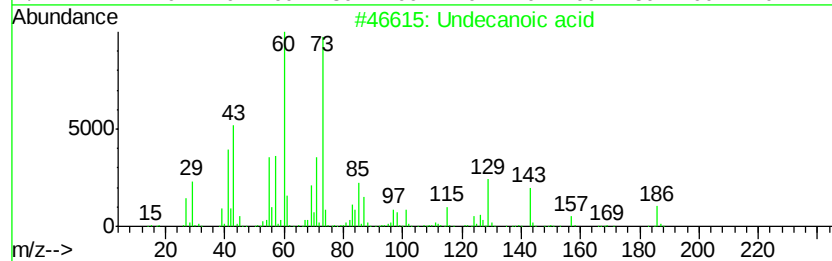
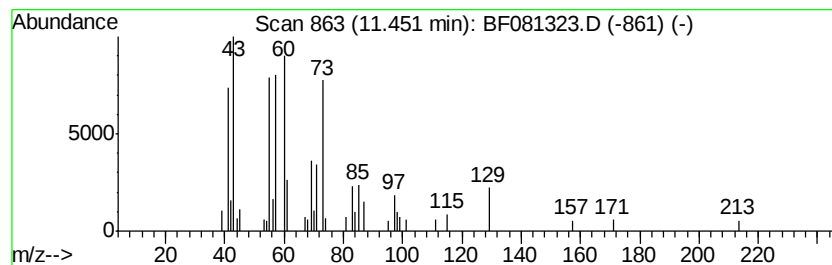
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Peak Number 4 Undecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.45	2.63 ng	67094	Phenanthrene-d10	10.88

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid		186	C11H22O2	000112-37-8	64
2	n-Decanoic acid		172	C10H20O2	000334-48-5	50
3	.alpha.-D-Glucopyranoside, .alph...		342	C12H22O11	000099-20-7	50
4	Octanoic Acid		144	C8H16O2	000124-07-2	47
5	n-Capric acid isopropyl ester		214	C13H26O2	002311-59-3	45



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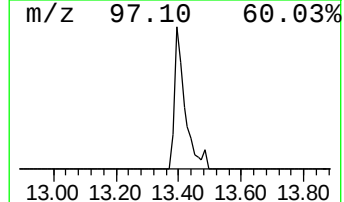
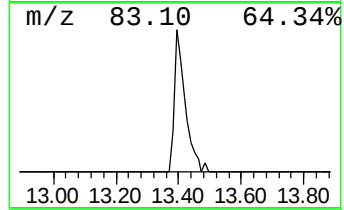
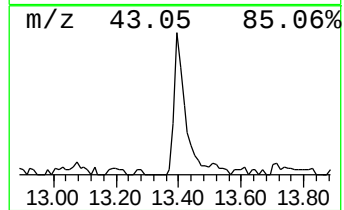
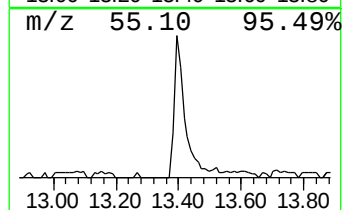
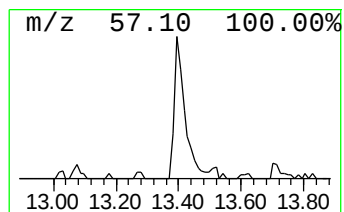
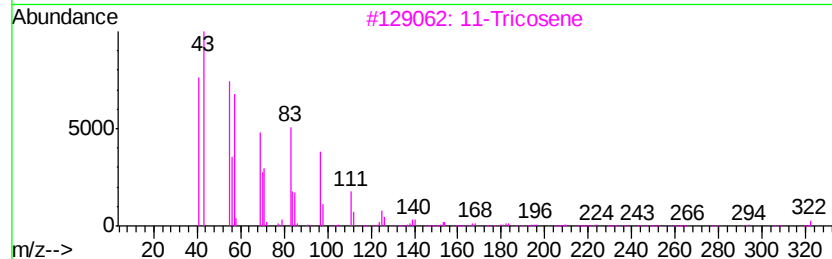
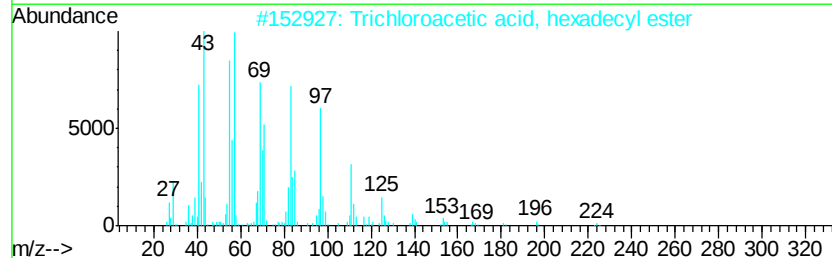
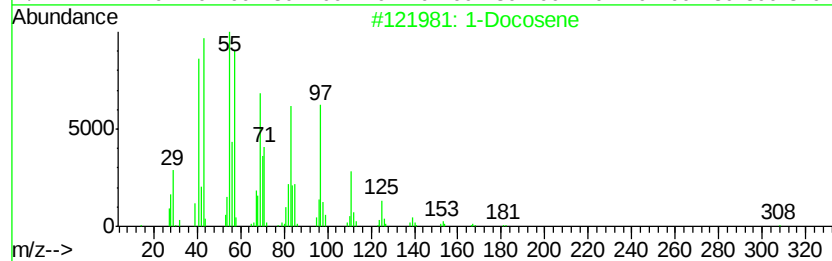
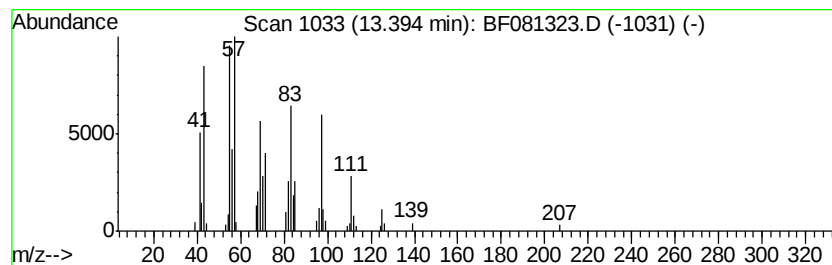
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Peak Number 5 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.39	9.52 ng	195251	Chrysene-d12	13.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	91
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3		11-Tricosene	322	C23H46	052078-56-5	86
4		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	83
5		1-Hexacosanol	382	C26H54O	000506-52-5	83



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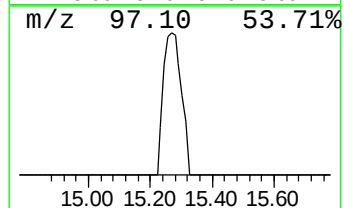
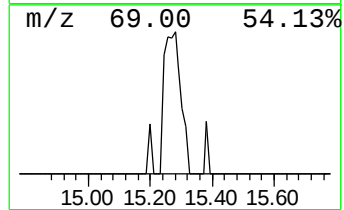
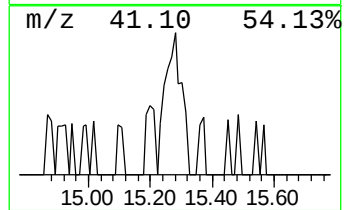
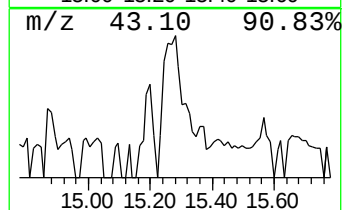
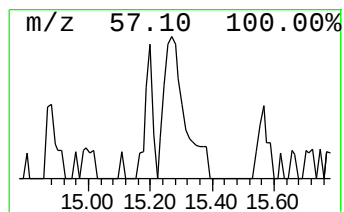
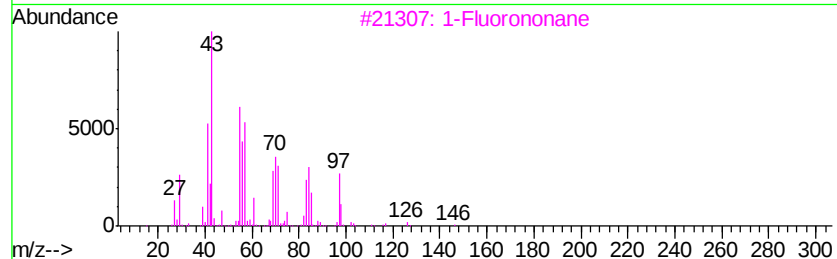
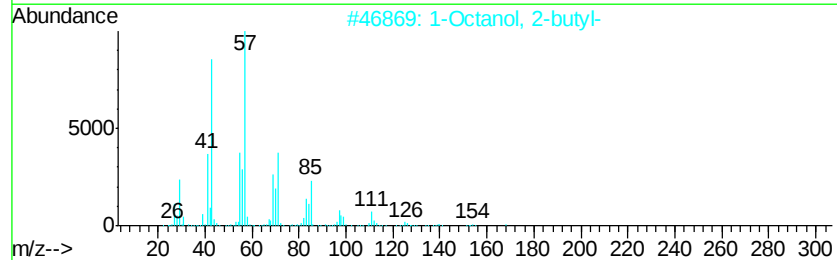
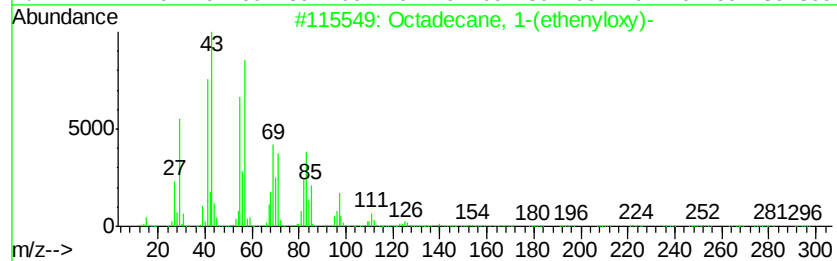
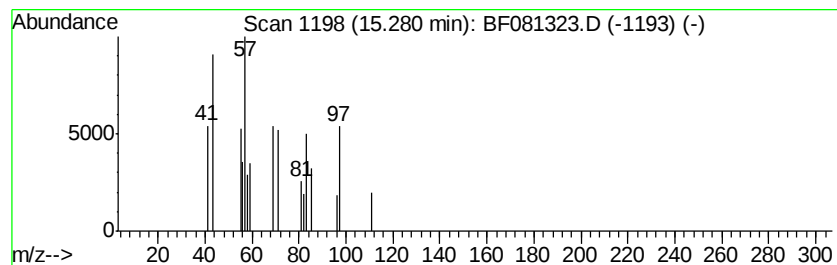
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Peak Number 6 unknown15.28 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.28	2.54 ng	40275	Perylene-d12	14.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	42
2		1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	37
3		1-Fluorononane	146	C9H19F	000463-18-3	28
4		1,3-Dimethylcyclopentanol	114	C7H14O	019550-46-0	12
5		2,5-Dimethyl-1-pyrroline	97	C6H11N	000822-64-0	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.46	65.0	ng	1195540	1	6.39	368120	20.0
unknown6.16	6.16	100.4	ng	1848340	1	6.39	368120	20.0
Undecanoic acid	11.45	2.6	ng	67094	4	10.88	510307	20.0
1-Docosene	13.39	9.5	ng	195251	5	13.49	410406	20.0
unknown15.28	15.28	2.5	ng	40275	6	14.80	317592	20.0