

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031517\
 Data File : BF093692.D
 Acq On : 16 Mar 2017 5:07
 Operator : SJ/MA
 Sample : PB97590BL
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB97590BL

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-BF030717.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	4.184	199	201	214	rBV	31760	100944	2.64%	0.327%
2	4.847	257	259	277	rBV	1467621	2238519	58.64%	7.247%
3	5.304	297	299	317	rBV2	1730208	3378884	88.51%	10.939%
4	6.367	390	392	400	rBV	2133831	3082260	80.74%	9.978%
5	6.482	400	402	405	rVB	2855707	2899708	75.96%	9.387%
6	6.710	420	422	428	rVB	692250	930141	24.37%	3.011%
7	6.859	433	435	438	rBV	3254438	3128555	81.95%	10.128%
8	7.282	470	472	482	rBV	2434079	2585178	67.72%	8.369%
9	8.002	532	535	537	rBV	1050092	1117699	29.28%	3.618%
10	9.076	627	629	632	rBV	2947738	3817447	100.00%	12.358%
11	9.762	686	689	691	rBV	792543	995066	26.07%	3.221%
12	10.551	756	758	766	rBV2	825275	1054278	27.62%	3.413%
13	11.248	817	819	824	rBV	927525	838960	21.98%	2.716%
14	12.654	939	942	944	rBV	42198	41160	1.08%	0.133%
15	12.837	955	958	960	rBV	2658473	2939069	76.99%	9.515%
16	13.888	1048	1050	1053	rBV	800802	810564	21.23%	2.624%
17	14.940	1137	1142	1146	rBV6	16861	40949	1.07%	0.133%
18	15.065	1146	1153	1157	rBV4	33899	145100	3.80%	0.470%
19	15.294	1170	1173	1178	rBV	548108	706277	18.50%	2.286%
20	16.105	1241	1244	1251	rVB2	18562	38654	1.01%	0.125%

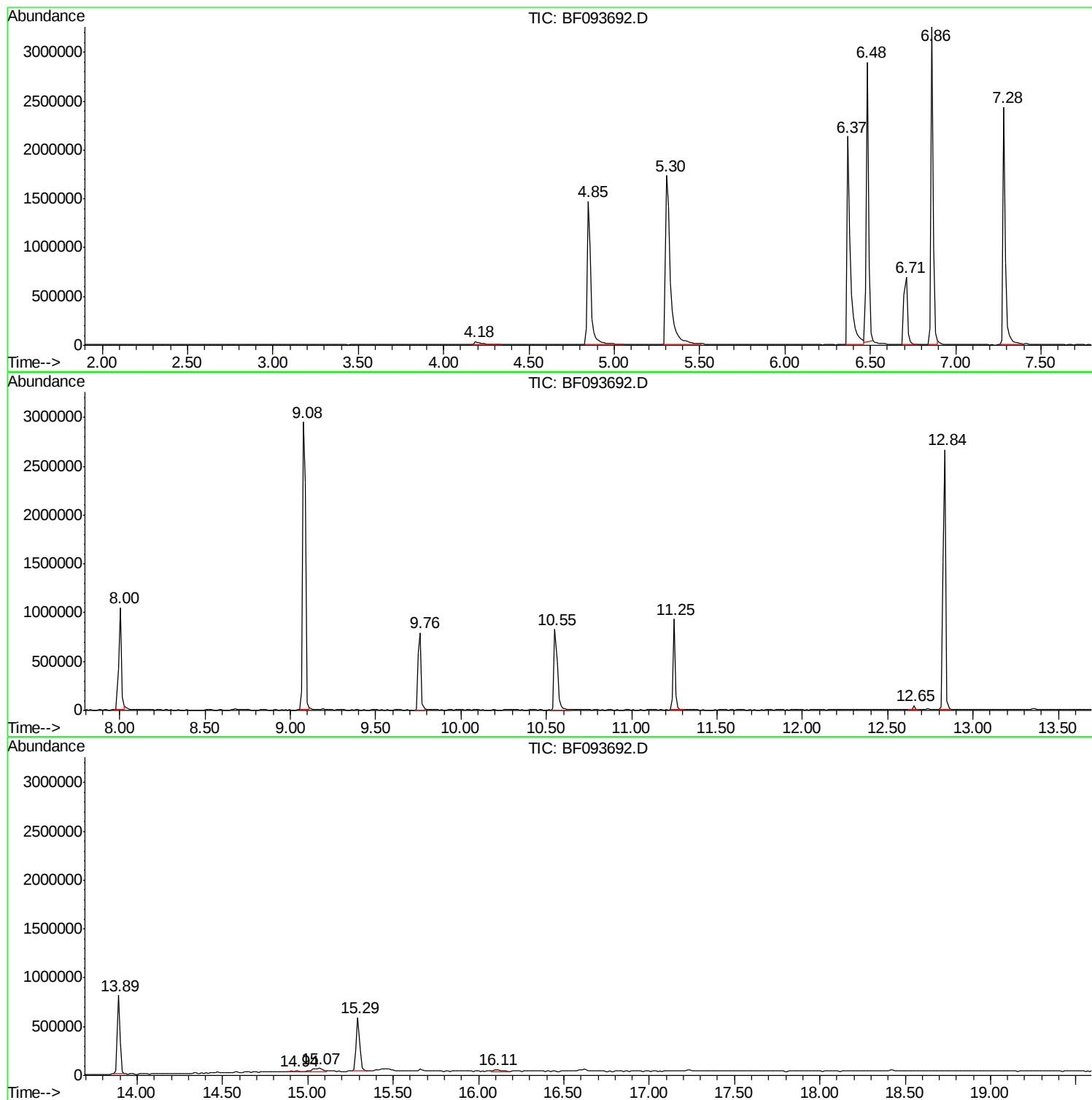
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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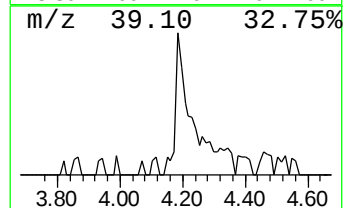
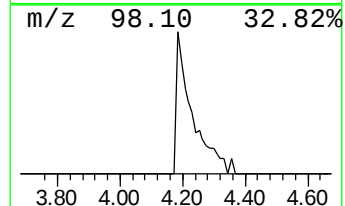
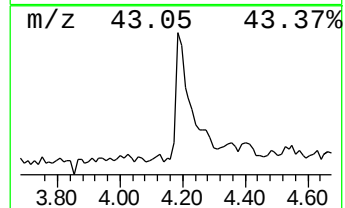
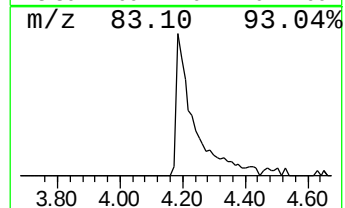
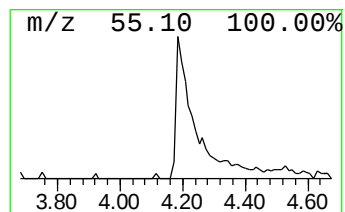
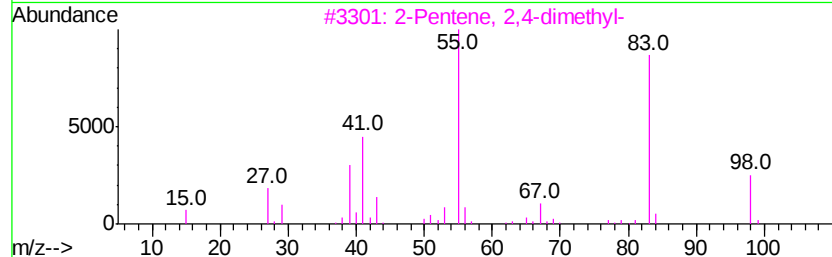
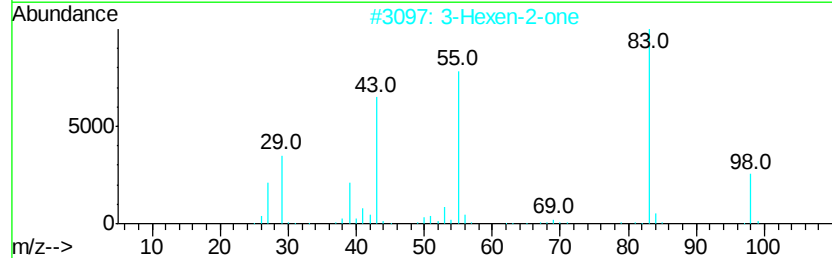
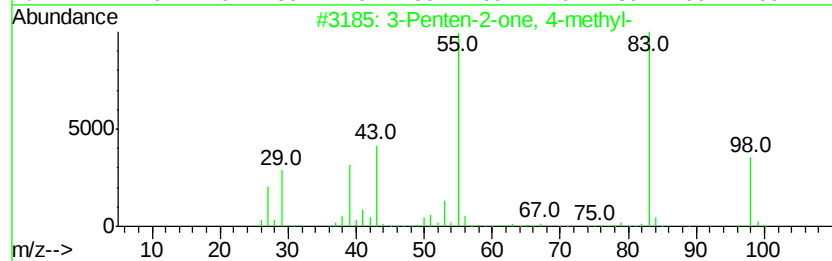
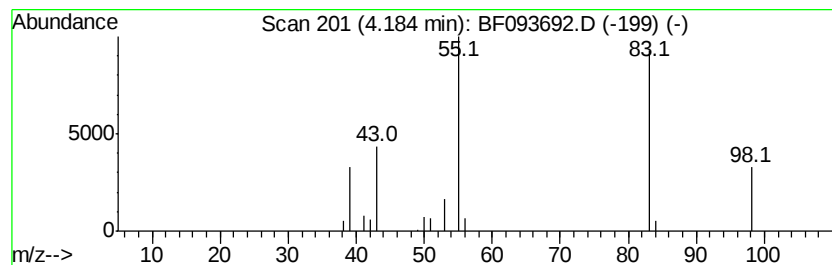
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.18	2.17 ng	100944	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	90
3		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78
5		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	72



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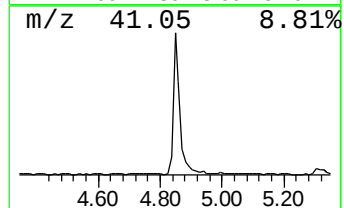
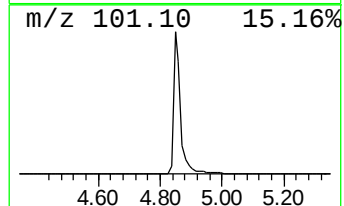
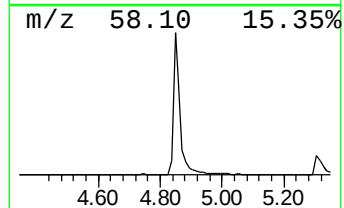
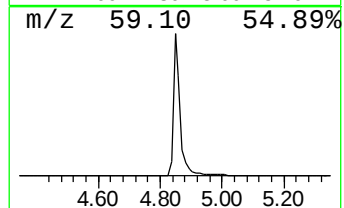
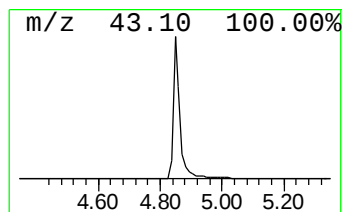
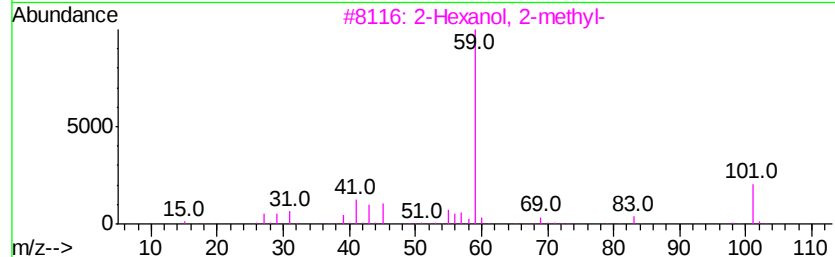
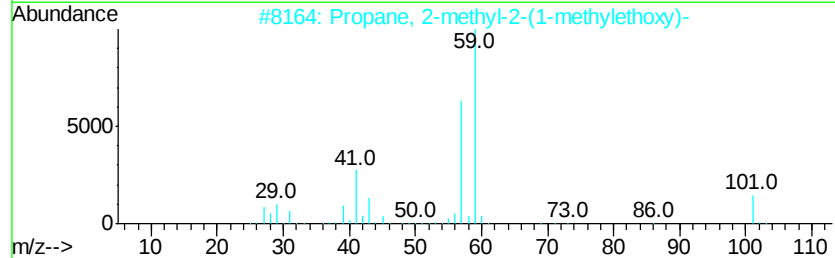
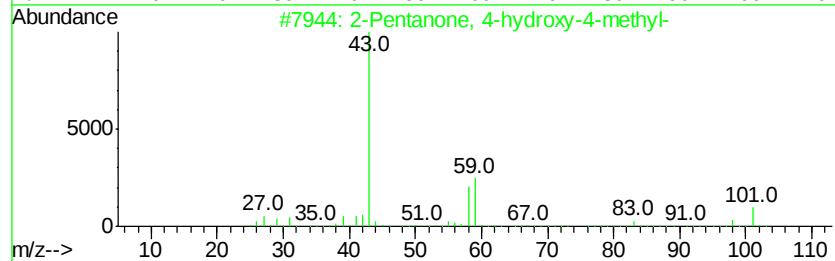
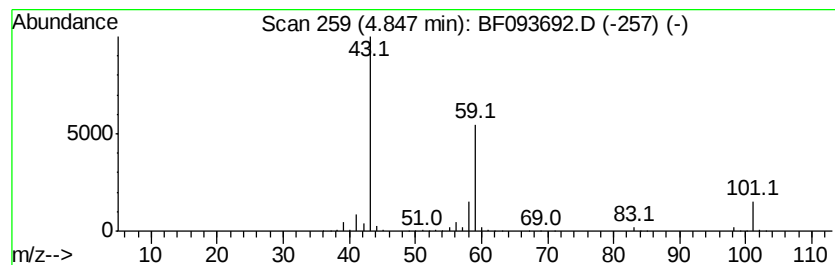
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	48.13 ng	2238520	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		Propane, 2-methyl-2-(1-methylethoxy)-	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-dimethyl-	141	C7H11NO2	001116-98-9	23



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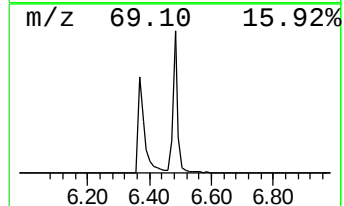
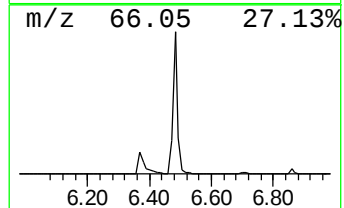
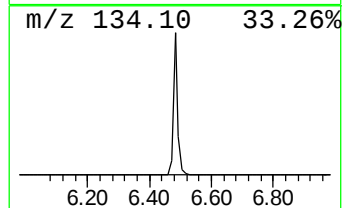
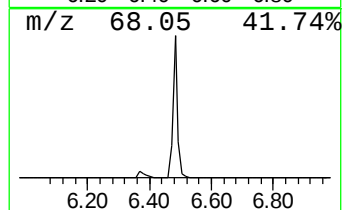
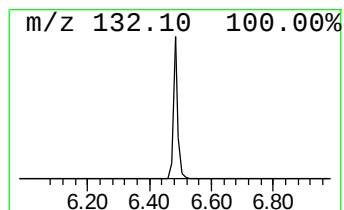
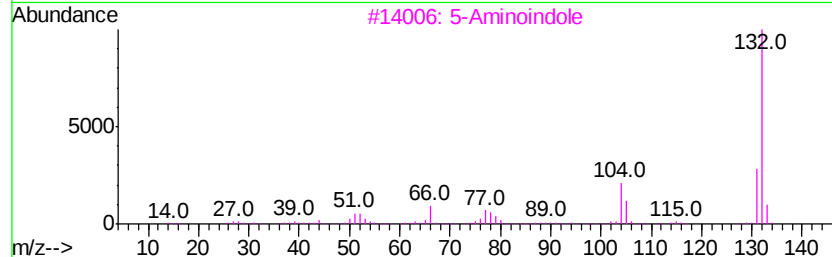
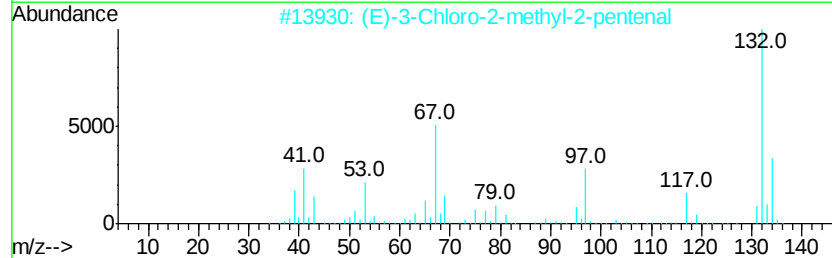
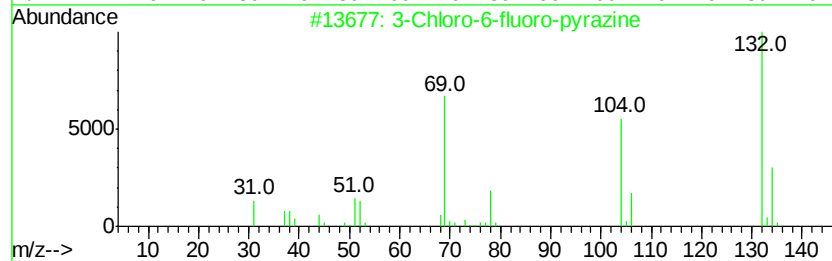
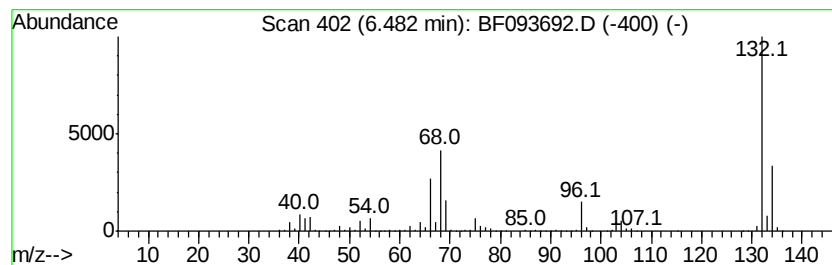
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Peak Number 3 unknown6.48 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	62.35 ng	2899710	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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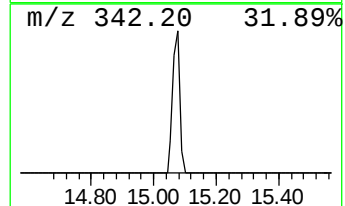
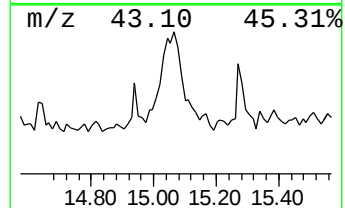
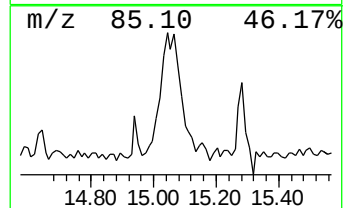
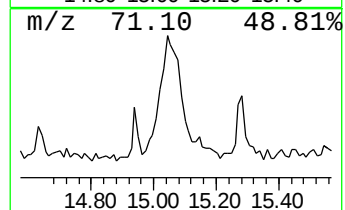
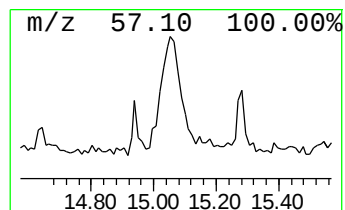
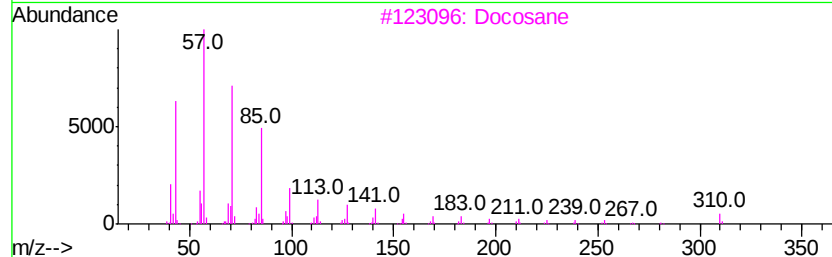
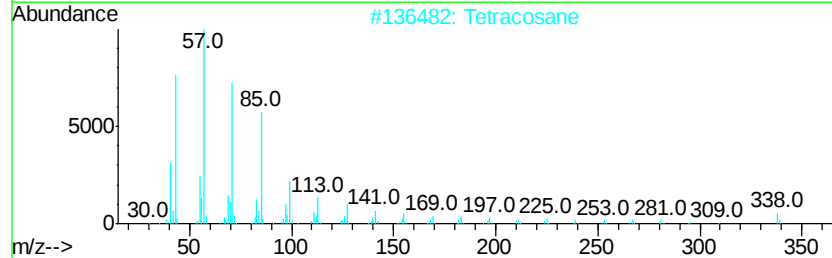
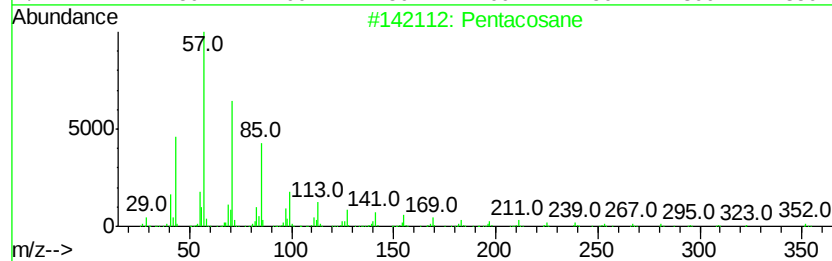
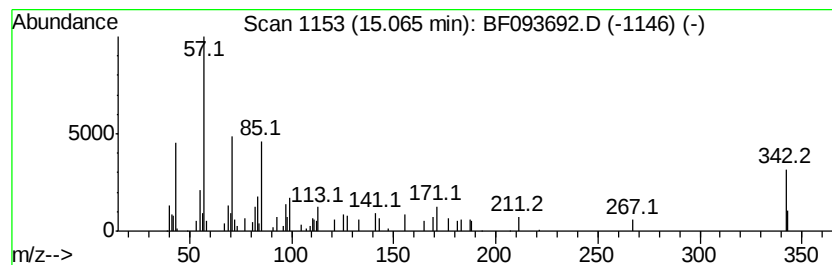
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Peak Number 5 Pentacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	4.11 ng	145100	Perylene-d12	15.29
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Pentacosane	352	C25H52	000629-99-2 58
2	Tetracosane	338	C24H50	000646-31-1 58
3	Docosane	310	C22H46	000629-97-0 58
4	Tricosane	324	C23H48	000638-67-5 58
5	Tetracosane, 11-decyl-	479	C34H70	055429-84-0 58



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.18	2.2	ng	100944	1	6.71	930141	20.0
2-Pentanone, 4-hy...	4.85	48.1	ng	2238520	1	6.71	930141	20.0
unknown6.48	6.48	62.4	ng	2899710	1	6.71	930141	20.0
Pentacosane	15.07	4.1	ng	145100	6	15.29	706277	20.0