

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022317\
 Data File : BF093114.D
 Acq On : 23 Feb 2017 19:49
 Operator : SJ/MA
 Sample : I1954-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CLP-S-04(10-15)

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-BF013017.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	5.013	253	256	271	rVB	1042923	1760934	40.81%	4.555%
2	5.436	290	293	296	rBV	3710291	3796082	87.97%	9.819%
3	6.476	381	384	387	rBV	3436958	3837683	88.93%	9.926%
4	6.602	393	395	398	rBV	3552503	3719477	86.19%	9.621%
5	6.830	413	415	418	rBV	892359	923966	21.41%	2.390%
6	6.990	427	429	432	rBV	3317320	2989650	69.28%	7.733%
7	7.402	462	465	468	rBV	2462526	2479426	57.46%	6.413%
8	7.516	473	475	480	rVB	33007	50694	1.17%	0.131%
9	8.122	525	528	530	rBV	1425080	1305777	30.26%	3.377%
10	9.196	619	622	625	rBV	3823377	4315356	100.00%	11.162%
11	9.596	655	657	659	rBV	694225	629475	14.59%	1.628%
12	9.802	672	675	679	rBV	39436	57851	1.34%	0.150%
13	9.870	679	681	684	rVB	1406068	1384282	32.08%	3.580%
14	10.305	715	719	721	rBV2	115462	123975	2.87%	0.321%
15	10.522	735	738	741	rBV	38818	63327	1.47%	0.164%
16	10.659	747	750	753	rBV2	1855917	2520101	58.40%	6.518%
17	10.773	758	760	765	rVB	160499	192470	4.46%	0.498%
18	11.219	797	799	801	rBV	95551	100844	2.34%	0.261%
19	11.356	809	811	813	rBV	1650550	1418335	32.87%	3.669%
20	11.653	835	837	839	rBV	41435	48413	1.12%	0.125%
21	12.945	947	950	952	rBV	4016143	3980277	92.24%	10.295%
22	13.837	1025	1028	1036	rBV	180629	286554	6.64%	0.741%
23	13.997	1039	1042	1044	rBV	1344772	1342833	31.12%	3.473%
24	14.831	1112	1115	1117	rBV	104932	138966	3.22%	0.359%
25	15.414	1164	1166	1177	rBV	693126	1100568	25.50%	2.847%
26	15.837	1200	1203	1206	rBV	27100	49827	1.15%	0.129%
27	16.317	1242	1245	1251	rVB2	21373	44622	1.03%	0.115%

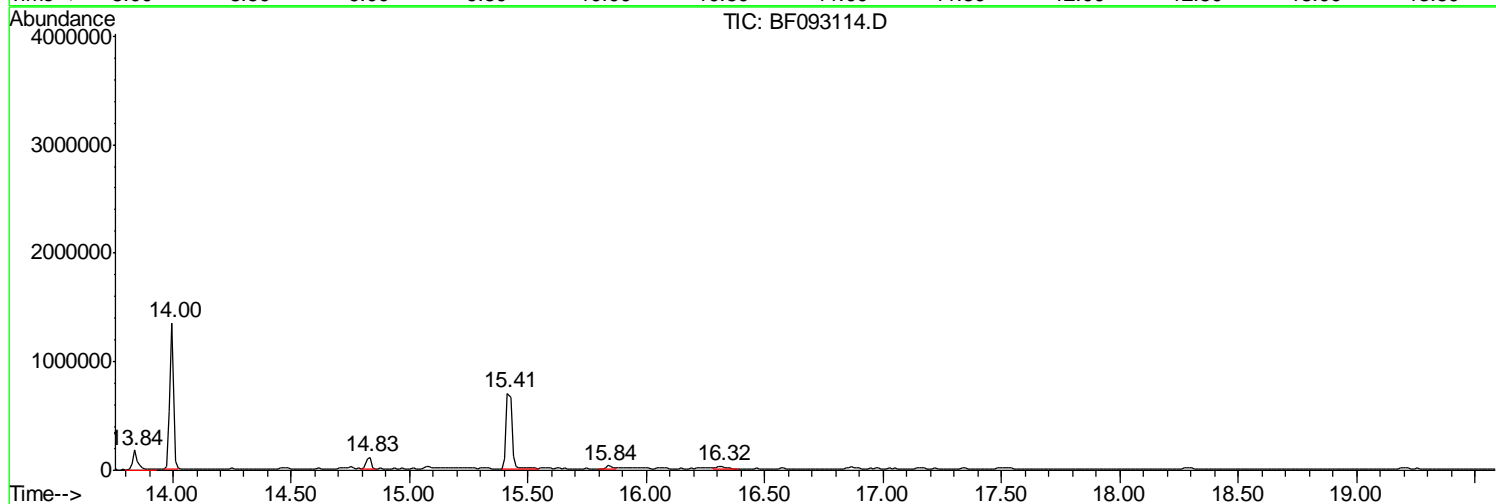
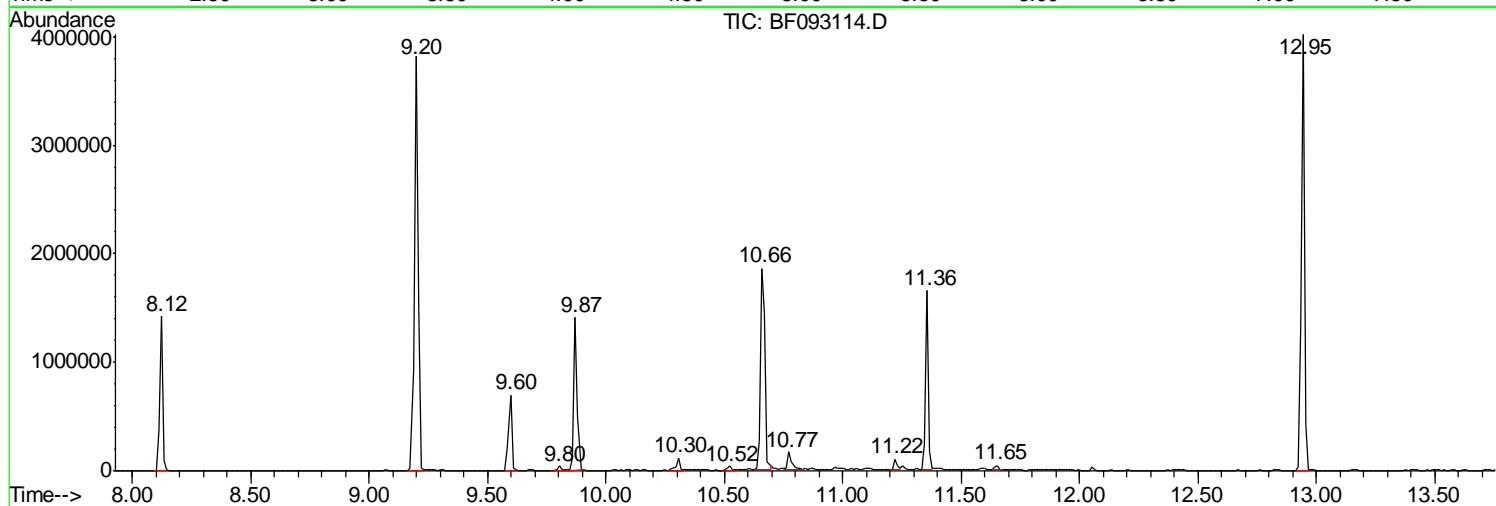
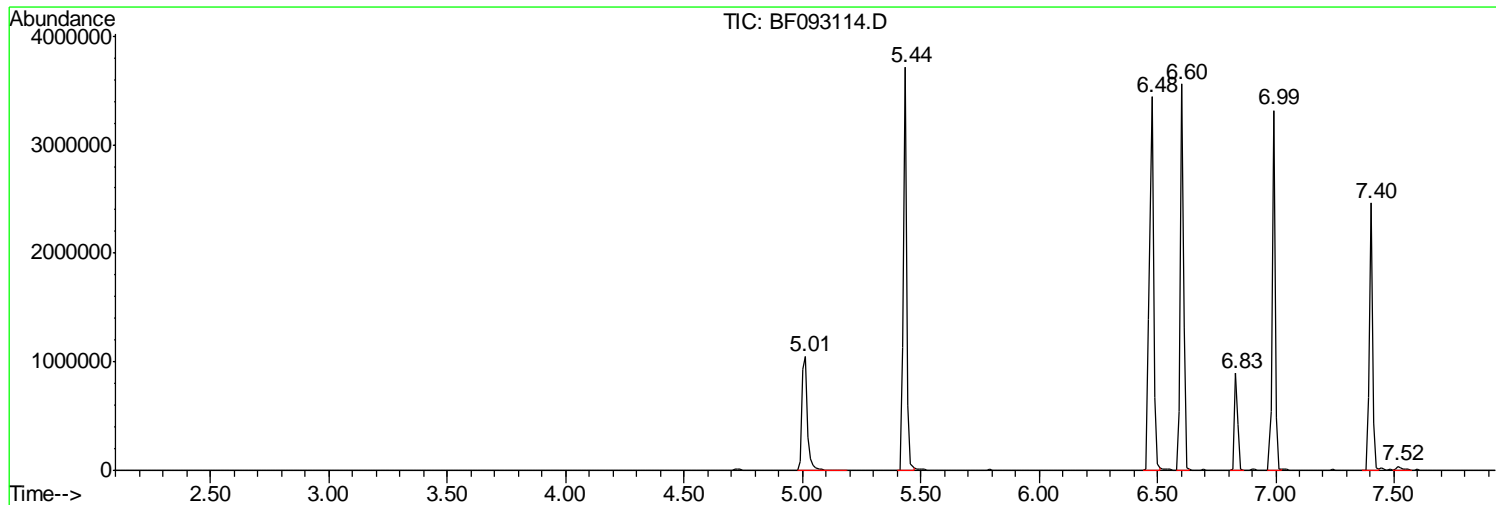
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ClientSampled :
CLP-S-04(10-15)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF013017.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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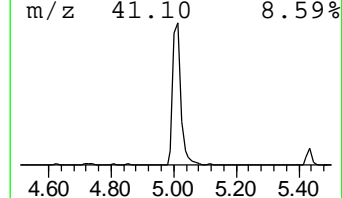
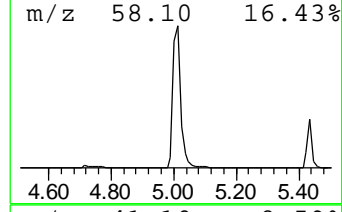
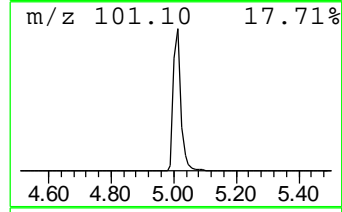
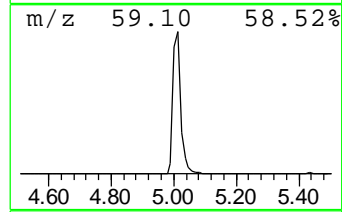
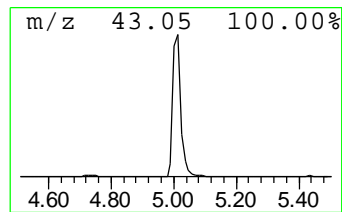
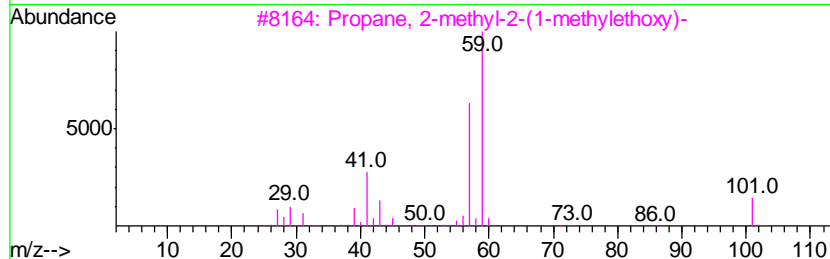
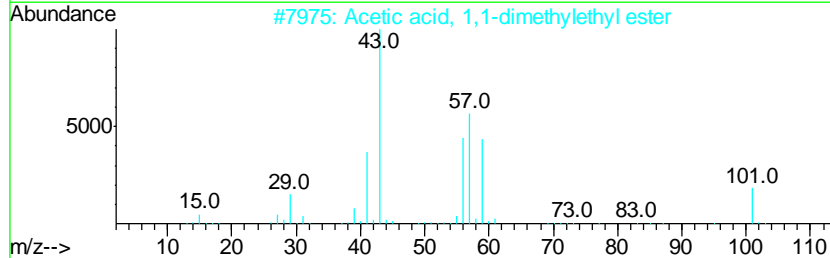
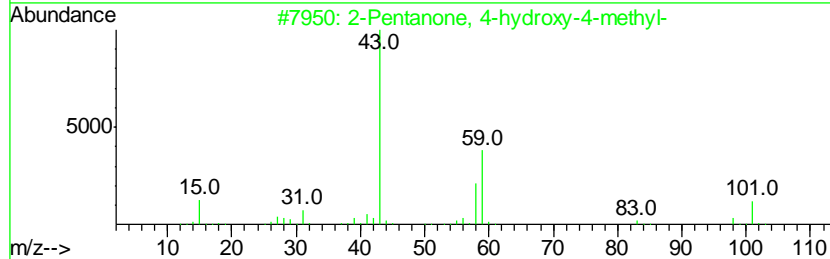
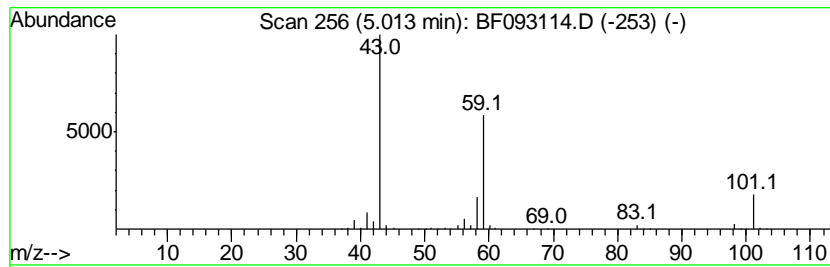
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TIC Library : C:\DATABASE\NIST02.L
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 Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	38.12 ng	1760930	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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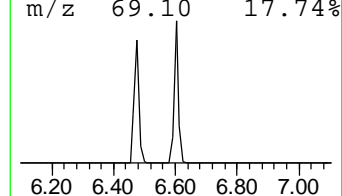
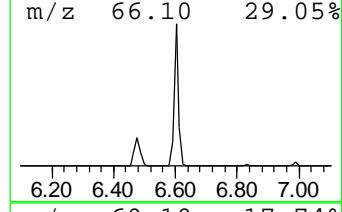
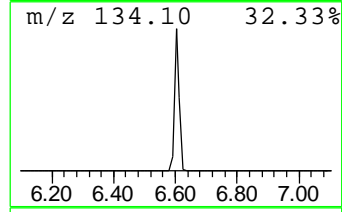
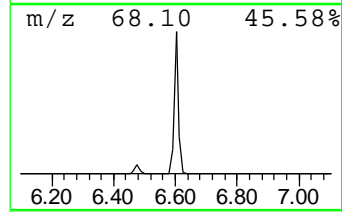
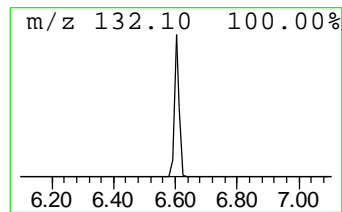
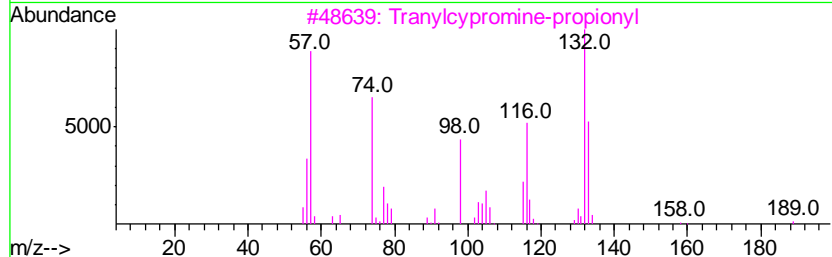
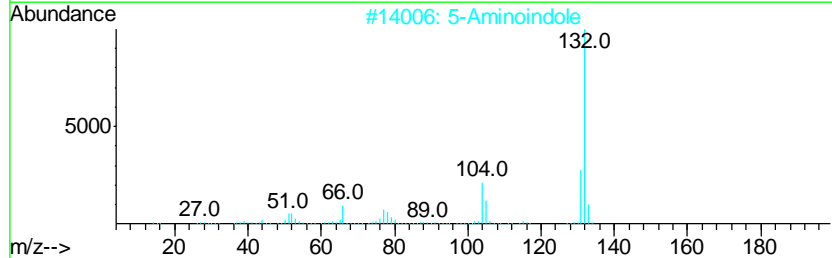
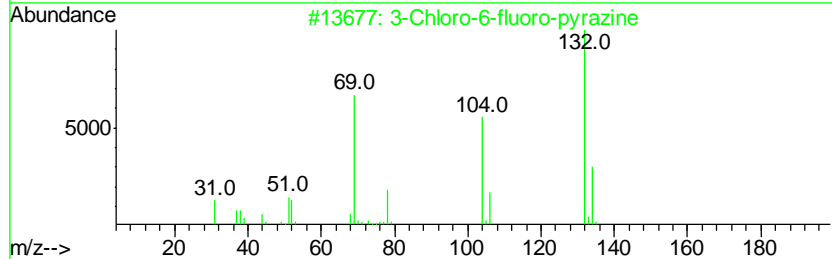
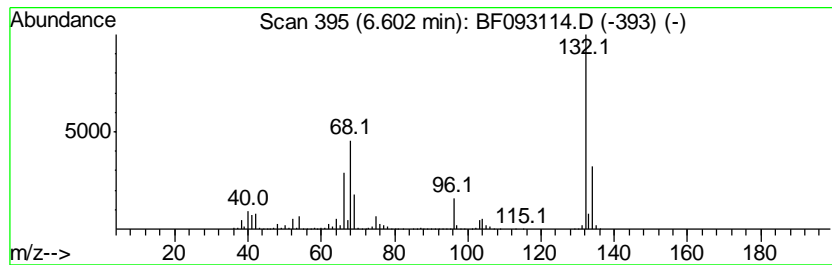
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 Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	80.51 ng	3719480	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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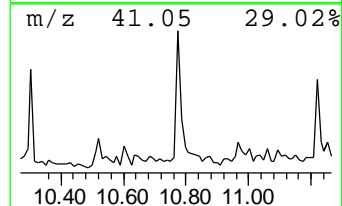
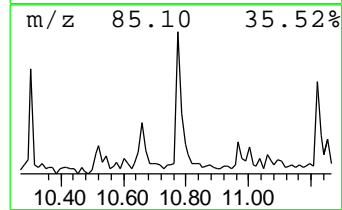
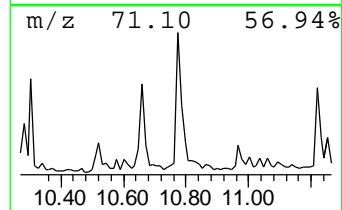
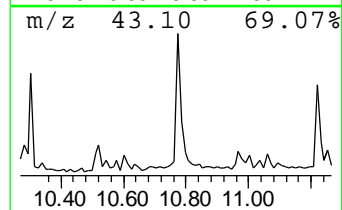
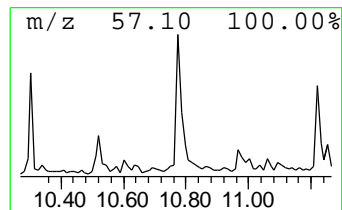
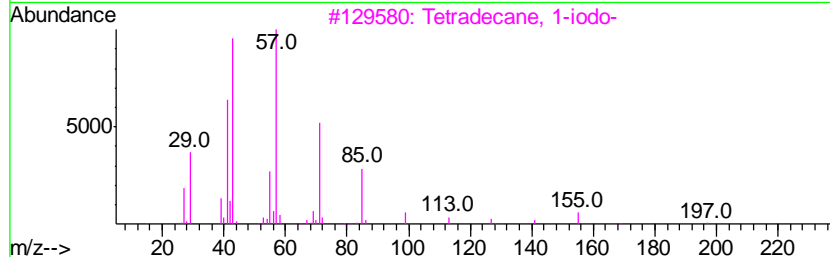
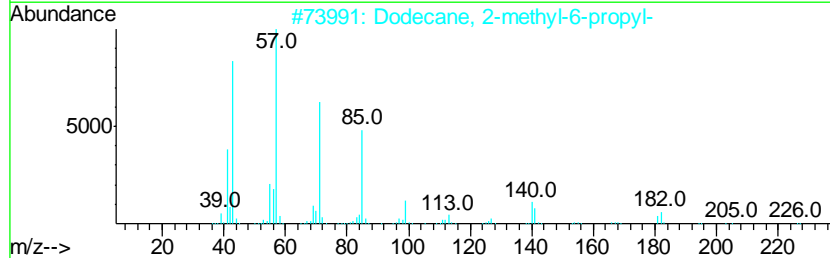
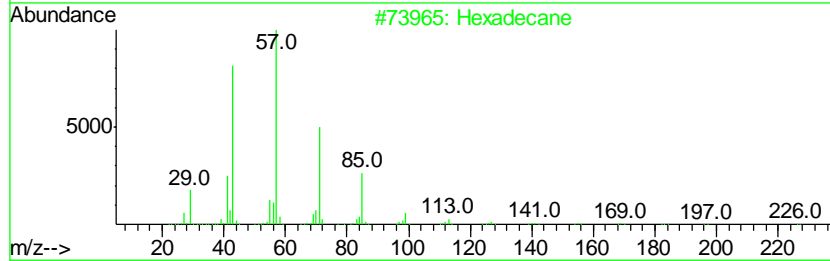
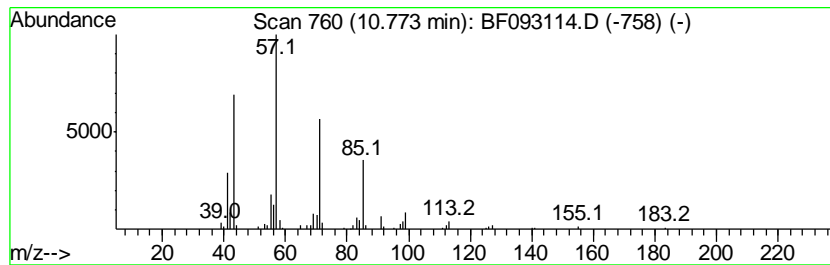
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 Peak Number 4 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.77	2.71 ng	192470	Phenanthrene-d10	11.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	91
2		Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86
3		Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
4		Tridecane	184	C13H28	000629-50-5	72
5		Pentadecane	212	C15H32	000629-62-9	72



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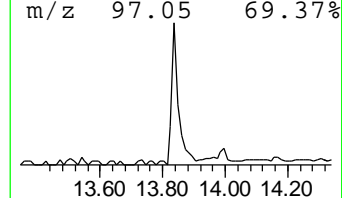
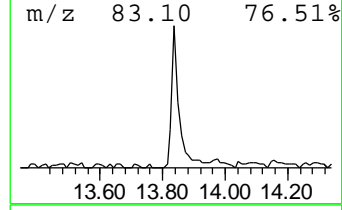
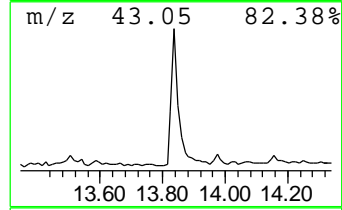
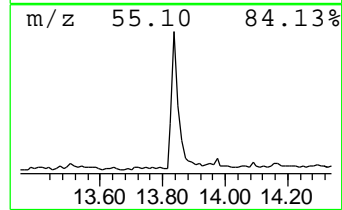
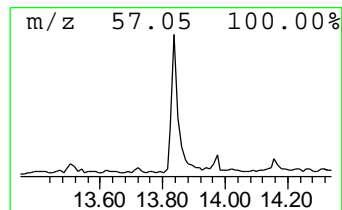
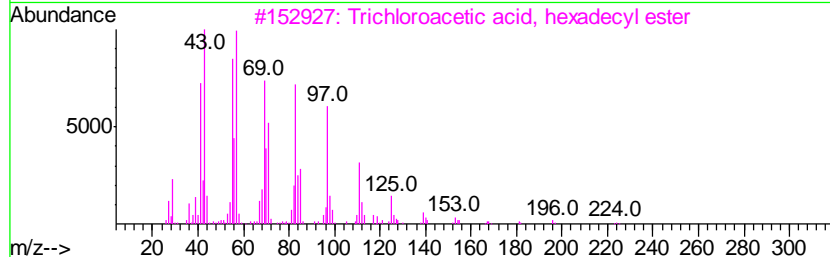
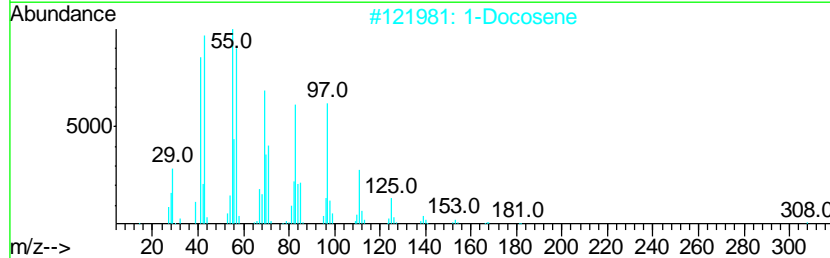
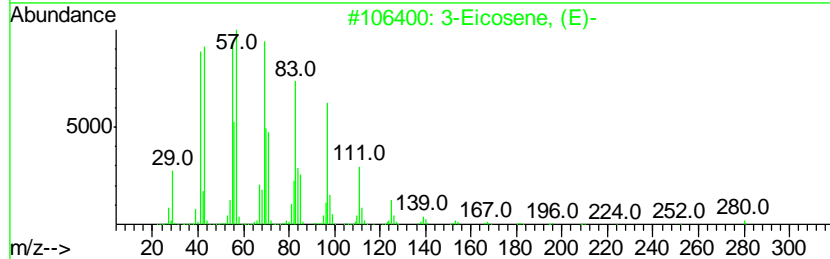
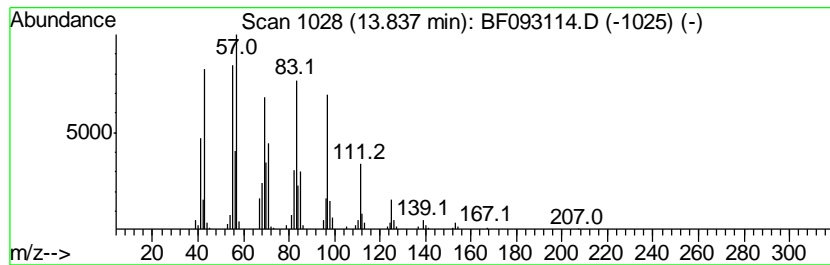
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 Peak Number 5 3-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	4.27 ng	286554	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
2		1-Docosene	308	C22H44	001599-67-3	91
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4		9-Eicosene, (E)-	280	C20H40	074685-29-3	91
5		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91



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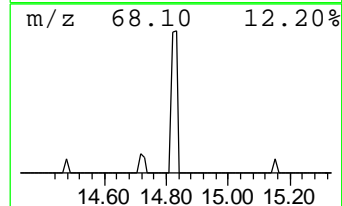
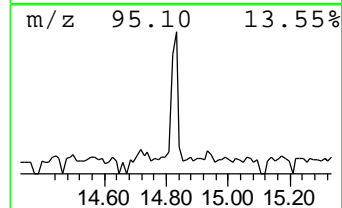
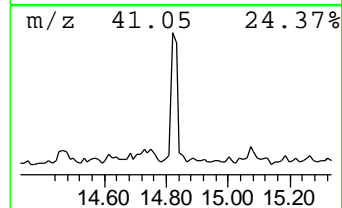
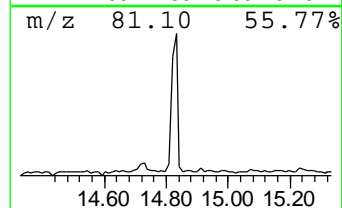
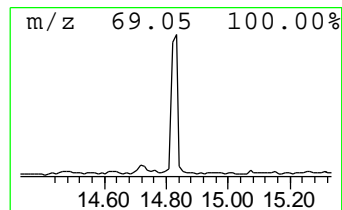
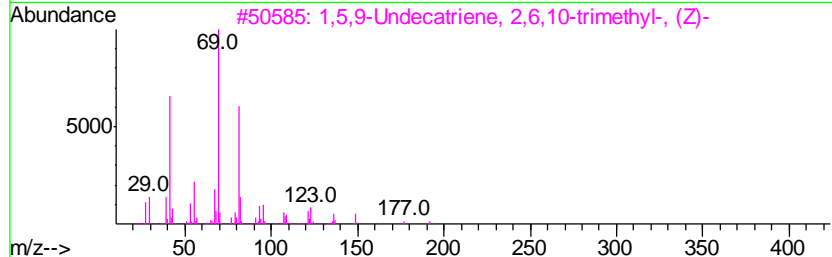
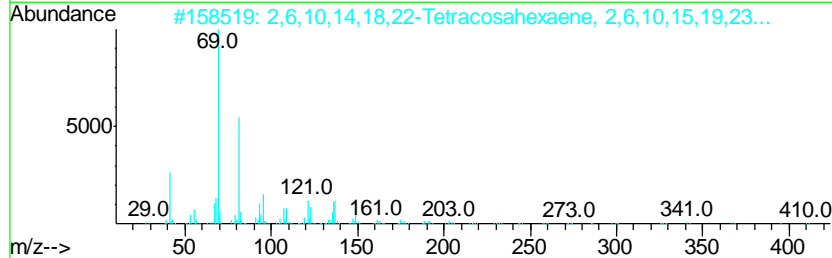
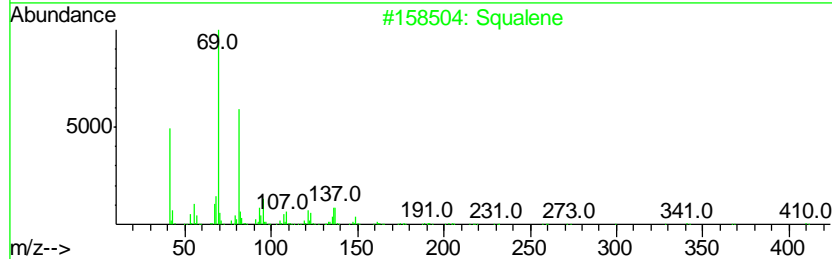
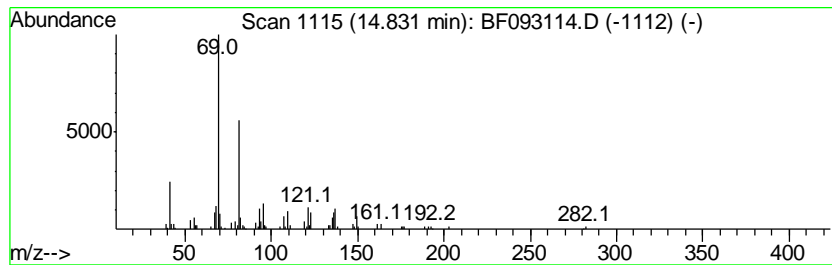
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 Peak Number 6 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	2.53 ng	138966	Perylene-d12	15.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	91
2		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	91
3		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
4		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	86
5		.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.01	38.1 ng		1760930	1	6.83	923966	20.0
unknown6.60	6.60	80.5 ng		3719480	1	6.83	923966	20.0
Hexadecane	10.77	2.7 ng		192470	4	11.36	1418340	20.0
3-Eicosene, (E)-	13.84	4.3 ng		286554	5	14.00	1342830	20.0
Squalene	14.83	2.5 ng		138966	6	15.43	1100570	20.0