

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012417\
 Data File : BF092439.D
 Acq On : 24 Jan 2017 20:00
 Operator : UM/SJ
 Sample : I1322-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B1-8-9

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-BF012417.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	5.150	265	268	271	rBV	981014	1127305	34.21%	3.721%
2	5.561	301	304	306	rBV	3016886	3221274	97.75%	10.633%
3	6.579	390	393	396	rBV	2418138	3116114	94.56%	10.286%
4	6.727	403	406	409	rBV	2956171	2880949	87.42%	9.509%
5	6.967	425	427	429	rBV	1109531	925400	28.08%	3.055%
6	7.127	438	441	443	rBV	2283295	2416334	73.32%	7.976%
7	7.527	473	476	479	rBV	1854486	1818079	55.17%	6.001%
8	8.259	537	540	542	rBV	1458891	1251809	37.99%	4.132%
9	9.345	632	635	637	rBV	3549068	3295453	100.00%	10.878%
10	9.619	657	659	661	rBV	44231	36770	1.12%	0.121%
11	9.733	667	669	671	rBV	157569	168371	5.11%	0.556%
12	10.031	692	695	697	rVB	1059081	1334939	40.51%	4.406%
13	10.465	729	733	734	rBV2	66979	70237	2.13%	0.232%
14	10.682	749	752	755	rBV	24280	34848	1.06%	0.115%
15	10.819	761	764	766	rBV	1539663	1877107	56.96%	6.196%
16	10.933	773	774	779	rVB	70515	99159	3.01%	0.327%
17	11.391	812	814	815	rBV	65246	56859	1.73%	0.188%
18	11.516	823	825	827	rBV	1525239	1288812	39.11%	4.254%
19	12.042	869	871	873	rBV	45129	52530	1.59%	0.173%
20	13.117	962	965	967	rBV	2333991	3116175	94.56%	10.286%
21	14.008	1041	1043	1051	rBV	123359	163144	4.95%	0.539%
22	14.157	1053	1056	1058	rBV	1189151	1054787	32.01%	3.482%
23	15.025	1130	1132	1134	rBV	103678	107746	3.27%	0.356%
24	15.631	1182	1185	1188	rBV	609396	747422	22.68%	2.467%
25	16.660	1271	1275	1278	rBV5	12883	34194	1.04%	0.113%

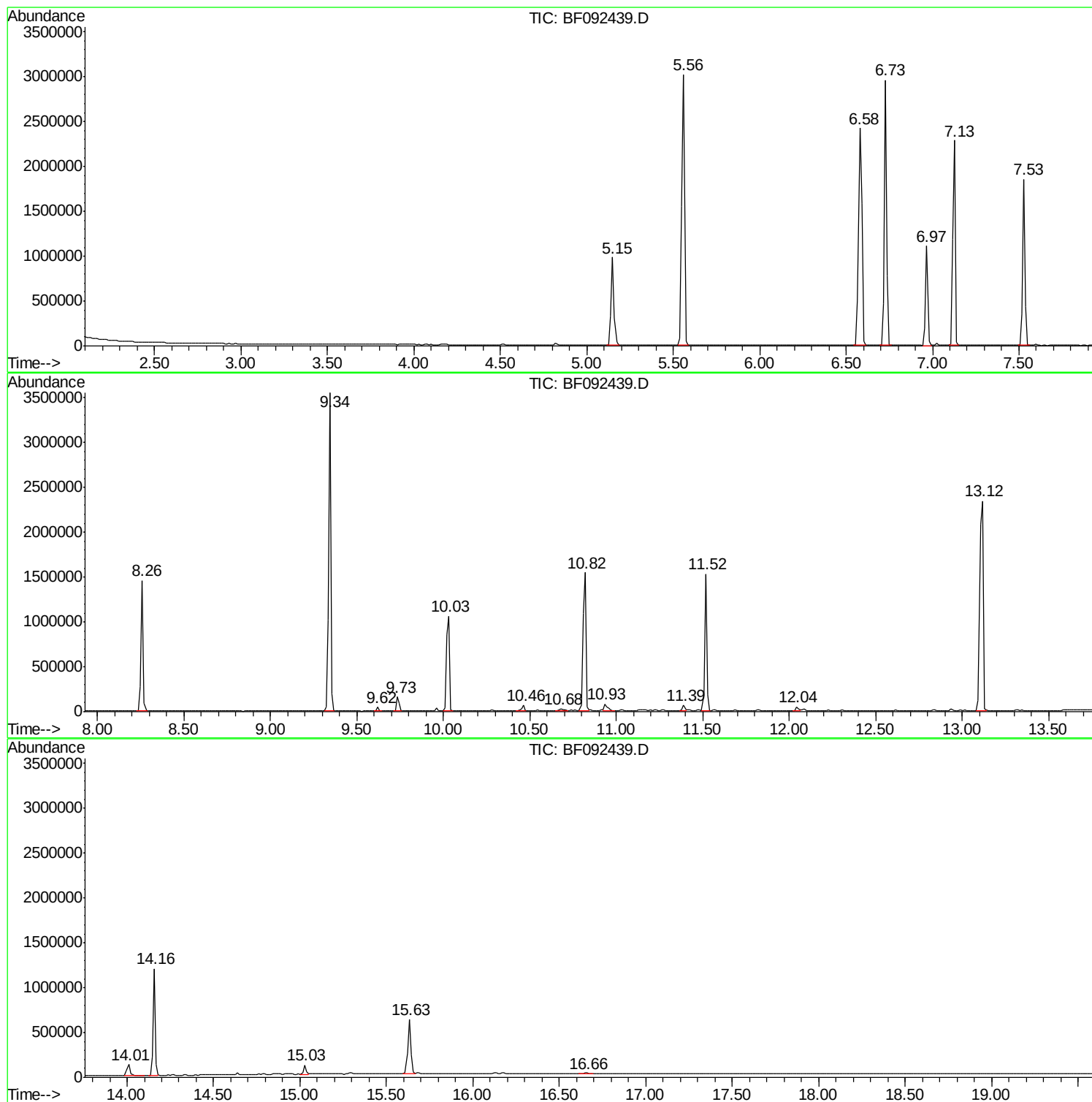
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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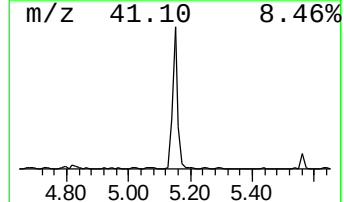
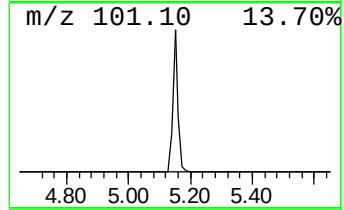
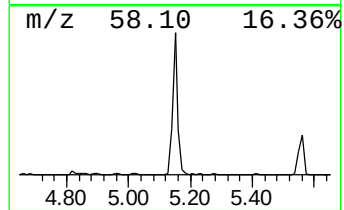
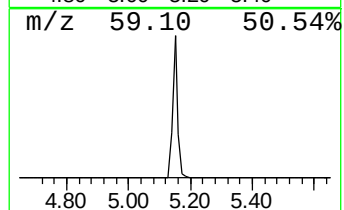
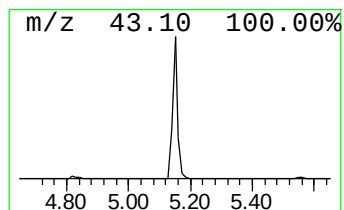
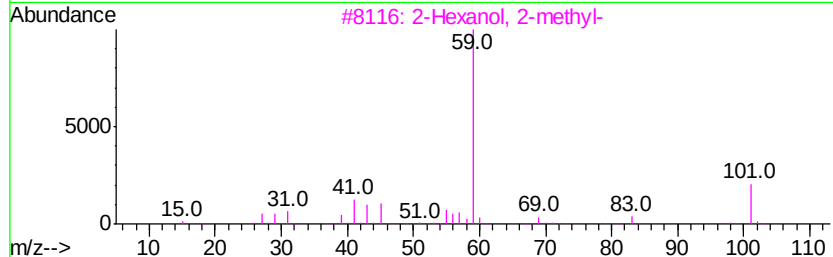
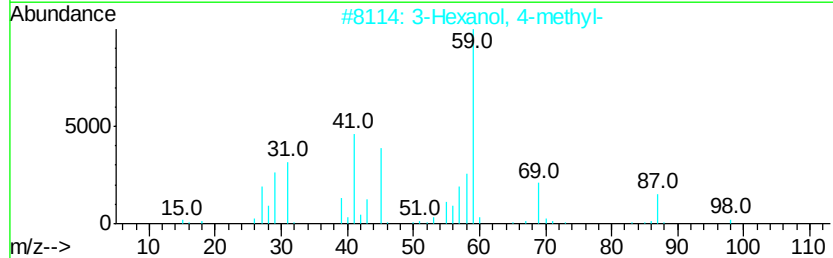
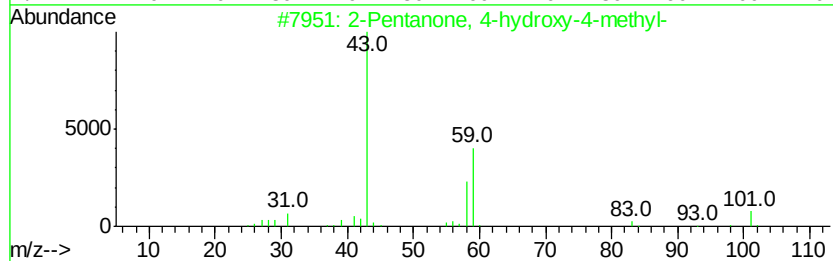
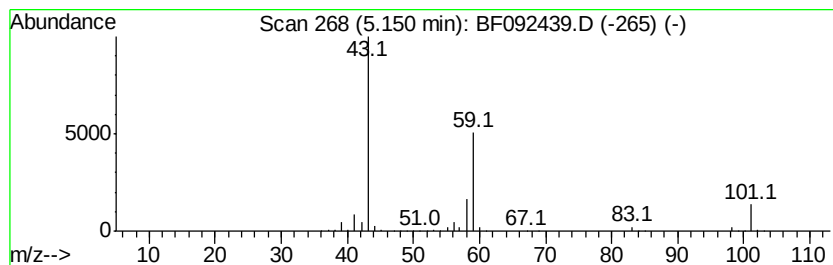
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.15	24.36 ng	1127310	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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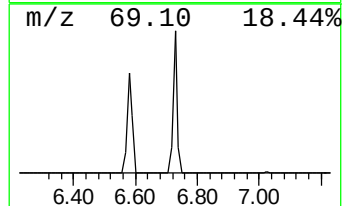
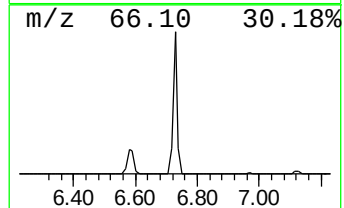
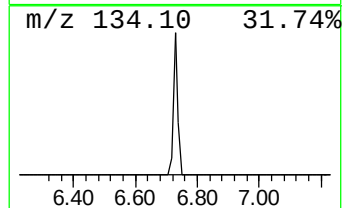
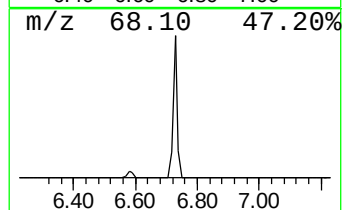
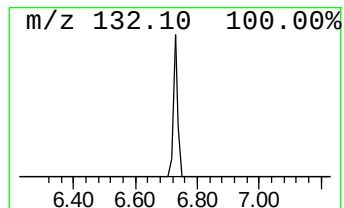
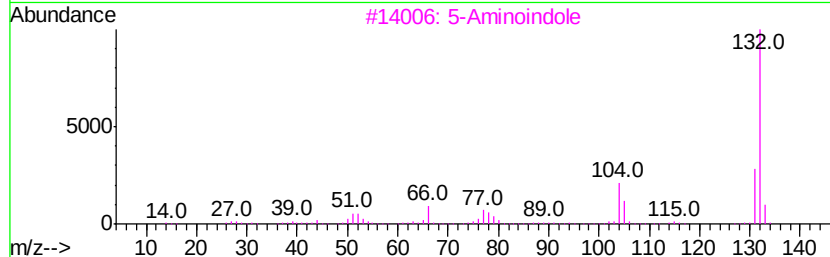
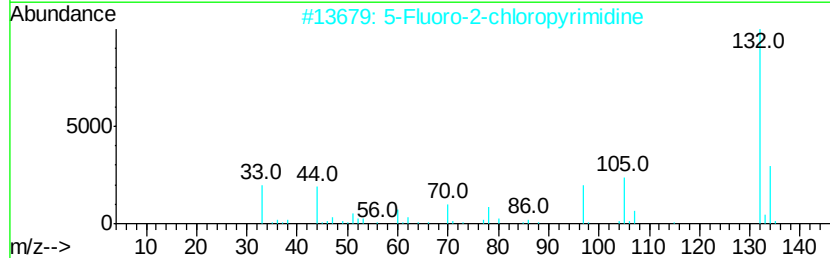
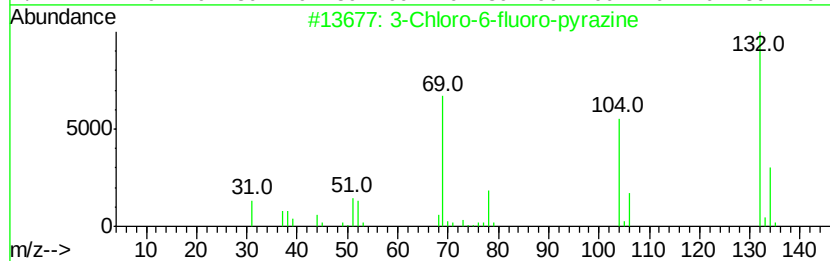
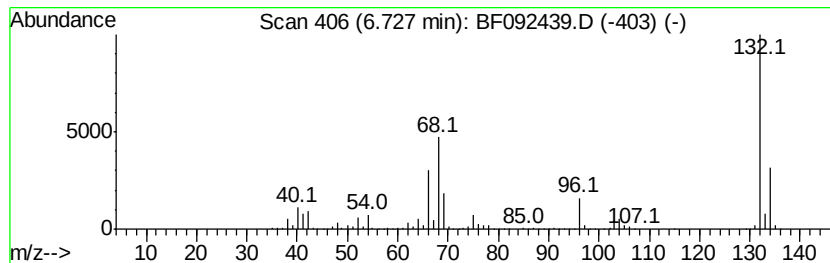
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Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	62.26 ng	2880950	1,4-Dichlorobenzene-d4	6.97

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		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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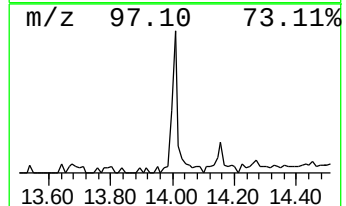
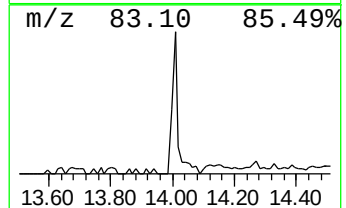
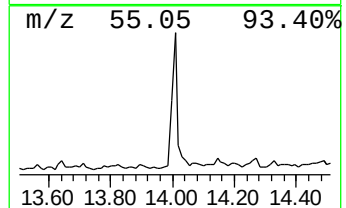
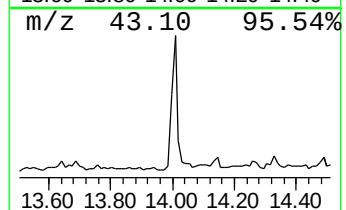
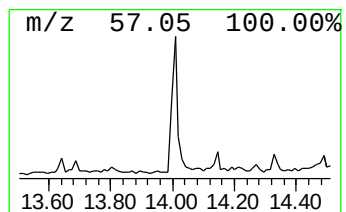
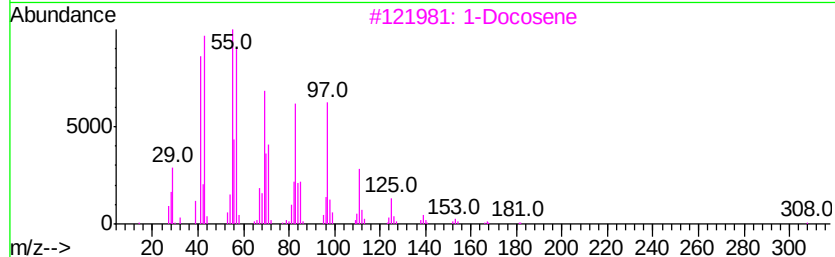
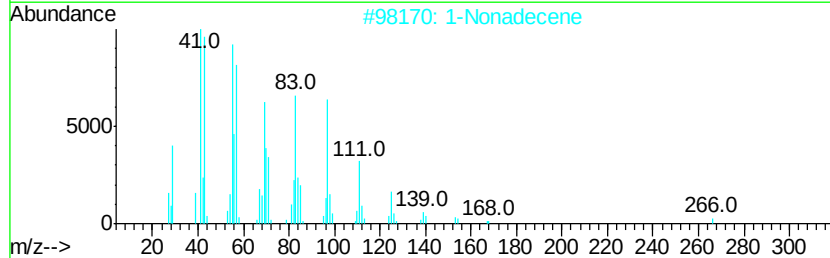
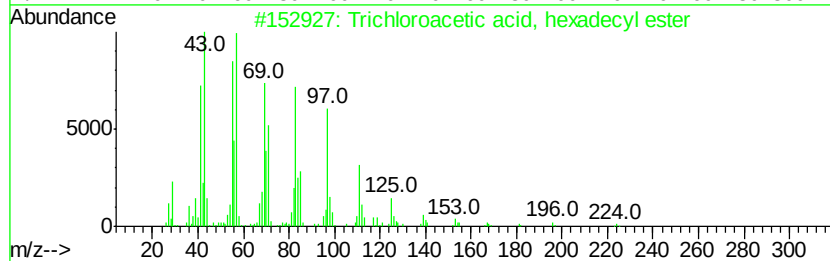
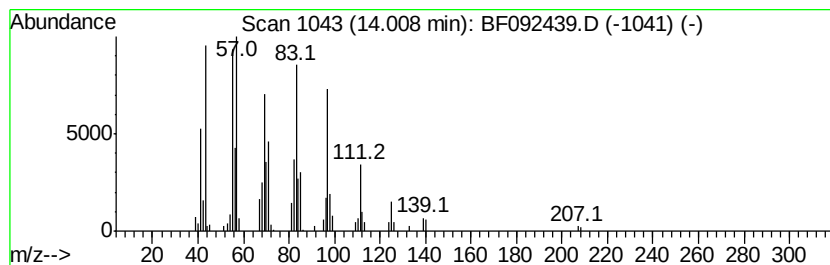
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Peak Number 4 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.01	3.09 ng	163144	Chrysene-d12	14.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2		1-Nonadecene	266	C19H38	018435-45-5	91
3		1-Docosene	308	C22H44	001599-67-3	91
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5		2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	91



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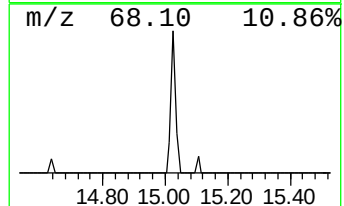
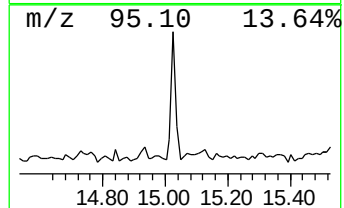
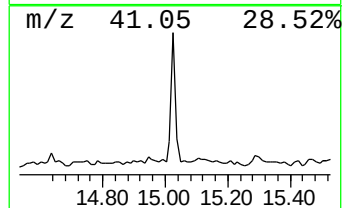
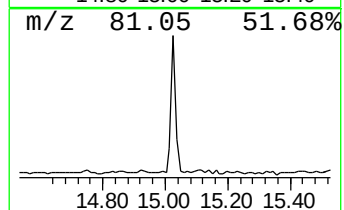
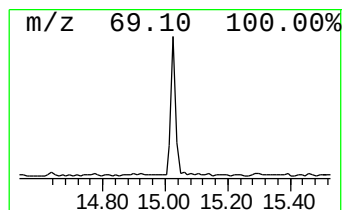
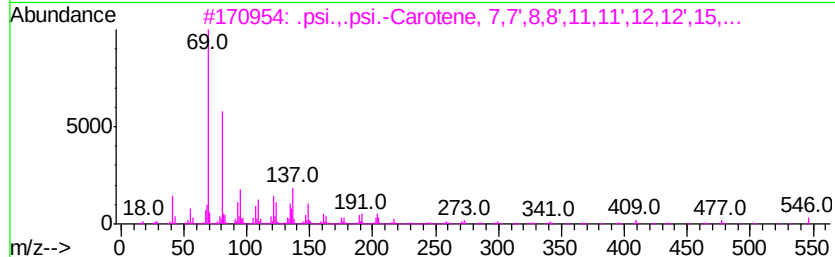
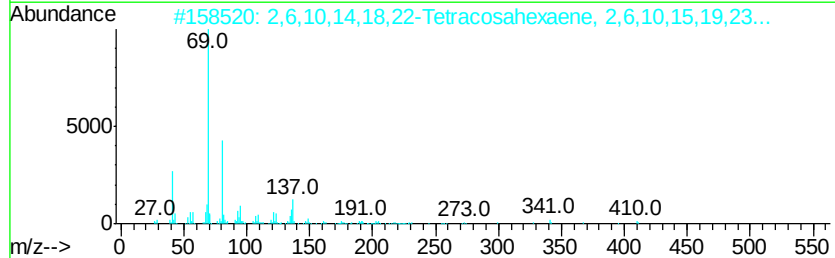
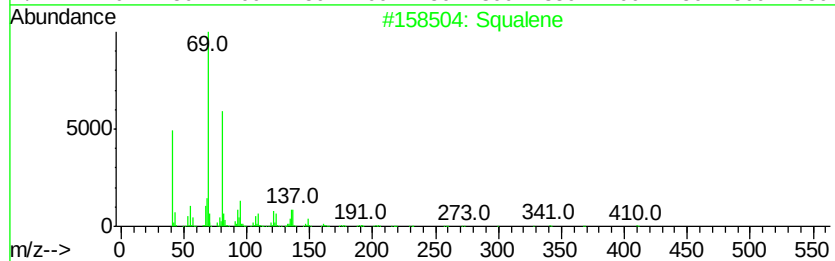
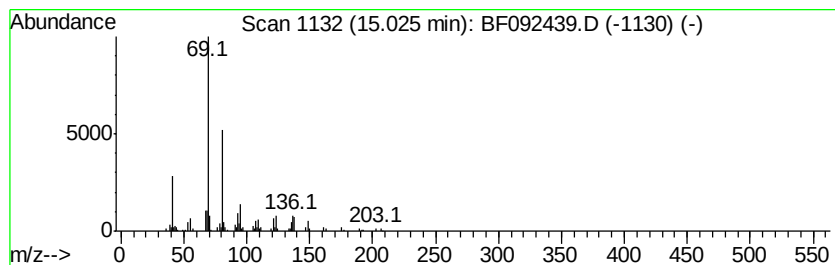
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Peak Number 5 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.03	2.88 ng	107746	Perylene-d12	15.63
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene		410 C30H50	007683-64-9 91
2	2,6,10,14,18,22-Tetracosahexaene...		410 C30H50	000111-02-4 90
3	.psi.,.psi.-Carotene, 7,7',8,8',...		547 C40H66	000502-62-5 83
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...		222 C15H26O	000106-28-5 78
5	5,9,13-Pentadecatrien-2-one, 6,1...		262 C18H30O	001117-52-8 72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.15	24.4	ng	1127310	1	6.97	925400	20.0
unknown6.73	6.73	62.3	ng	2880950	1	6.97	925400	20.0
Trichloroacetic a...	14.01	3.1	ng	163144	5	14.16	1054790	20.0
Squalene	15.03	2.9	ng	107746	6	15.63	747422	20.0