

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021115\
 Data File : BF077266.D
 Acq On : 11 Feb 2015 22:10
 Operator : TP/IZ
 Sample : G1273-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RU-1

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.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	1.287	32	35	39	rBV	7259	14122	1.76%	0.201%
2	1.344	39	40	55	rVB	121093	222104	27.70%	3.159%
3	3.539	229	232	250	rBB	68329	184699	23.04%	2.627%
4	4.544	317	320	340	rBV	256168	582533	72.66%	8.286%
5	6.967	529	532	535	rBV	338502	555494	69.28%	7.901%
6	7.036	535	538	548	rVB	393932	712673	88.89%	10.137%
7	7.539	580	582	590	rBB	85737	158021	19.71%	2.248%
8	7.859	607	610	620	rBB	287543	479130	59.76%	6.815%
9	8.853	694	697	710	rBV	234524	382547	47.71%	5.441%
10	10.453	834	837	846	rBB	140602	221385	27.61%	3.149%
11	11.939	965	967	973	rBB	15925	27593	3.44%	0.392%
12	13.105	1066	1069	1073	rBV	452922	744865	92.90%	10.595%
13	14.191	1161	1164	1169	rBB	25210	43574	5.43%	0.620%
14	14.568	1194	1197	1202	rBB	154692	254116	31.69%	3.614%
15	15.894	1311	1313	1316	rBB	6770	9974	1.24%	0.142%
16	16.283	1344	1347	1349	rBV	79565	105217	13.12%	1.497%
17	16.340	1349	1352	1358	rVB	274223	453774	56.60%	6.454%
18	17.471	1448	1451	1454	rBV	198958	258799	32.28%	3.681%
19	19.632	1638	1640	1645	rBV	28635	38160	4.76%	0.543%
20	19.723	1645	1648	1651	rVB	800955	801761	100.00%	11.404%
21	20.980	1756	1758	1762	rBV	258016	305174	38.06%	4.341%
22	21.129	1769	1771	1774	rBB	15303	21136	2.64%	0.301%
23	21.392	1791	1794	1797	rBB	6883	8497	1.06%	0.121%
24	21.780	1824	1828	1832	rBV	5791	9832	1.23%	0.140%
25	22.146	1857	1860	1862	rBV	5705	8263	1.03%	0.118%
26	22.203	1862	1865	1867	rVB	31883	41599	5.19%	0.592%
27	22.500	1888	1891	1893	rBV	6773	10386	1.30%	0.148%
28	22.615	1898	1901	1906	rVB	192862	244257	30.47%	3.474%
29	23.209	1950	1953	1954	rBV	6527	10175	1.27%	0.145%
30	23.243	1954	1956	1959	rVB3	5288	12898	1.61%	0.183%
31	23.369	1964	1967	1973	rBV4	4491	12908	1.61%	0.184%
32	23.495	1973	1978	1981	rBV6	3965	12550	1.57%	0.179%
33	23.563	1981	1984	1988	rBV4	7338	17270	2.15%	0.246%
34	23.918	2013	2015	2018	rBV4	3933	8963	1.12%	0.127%

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35	24.089	2027	2030	2033	rBV4	8383	16604	2.07%	0.236%
36	24.329	2048	2051	2054	rVB3	4362	9351	1.17%	0.133%
37	25.346	2137	2140	2144	rVB5	4034	10003	1.25%	0.142%
38	26.078	2201	2204	2208	rVB4	7690	20105	2.51%	0.286%

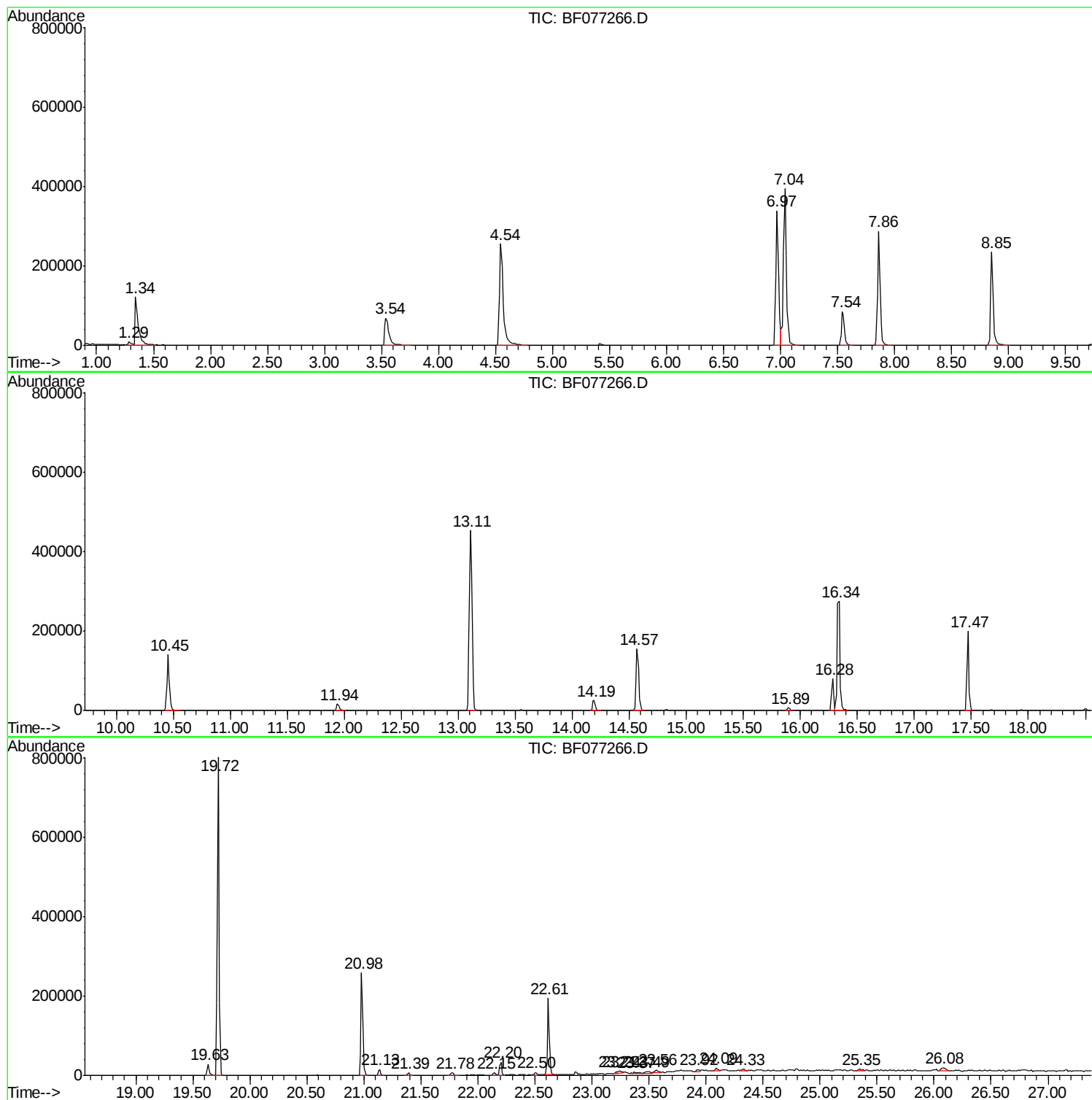
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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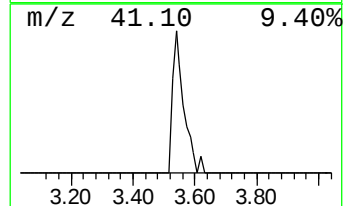
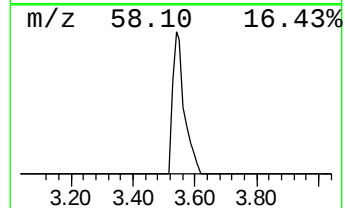
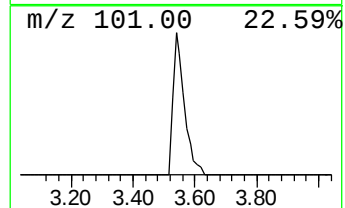
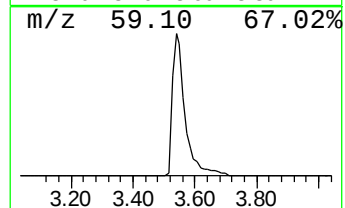
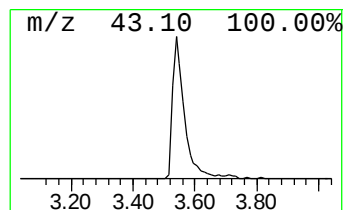
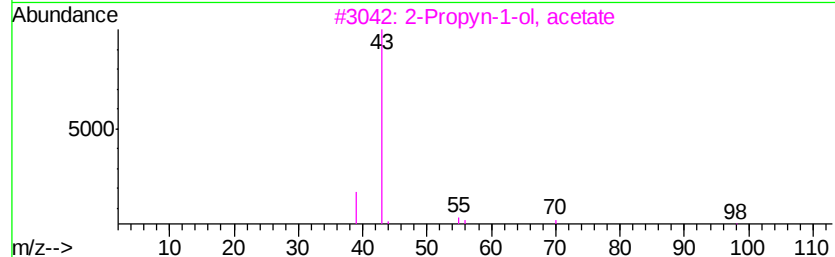
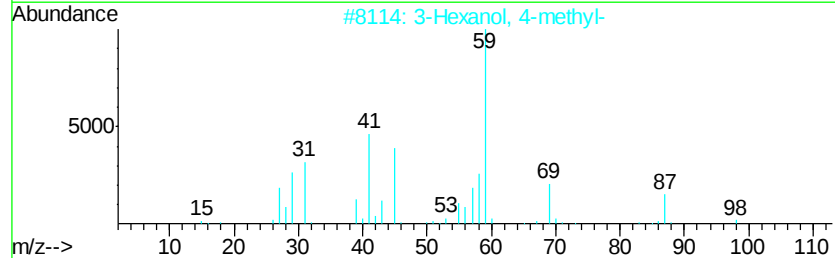
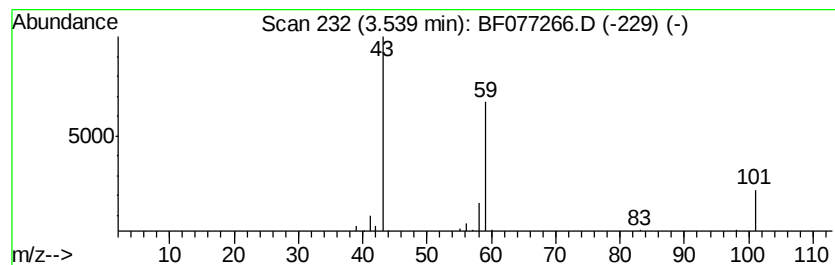
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.54	23.38 ng	184699	1,4-Dichlorobenzene-d4	7.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3		2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
4		2-Nonanone	142	C9H18O	000821-55-6	9
5		t-Butyl ethyl ether	102	C6H14O	1000118-18-4	9



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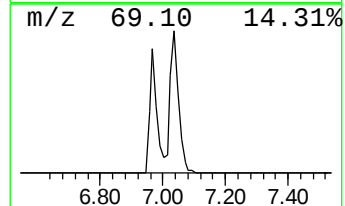
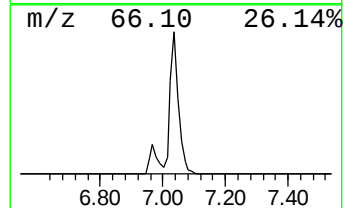
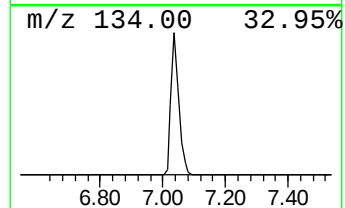
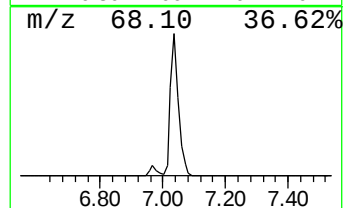
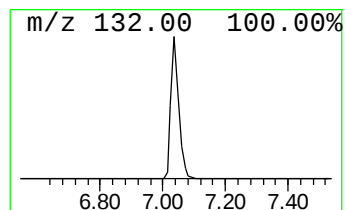
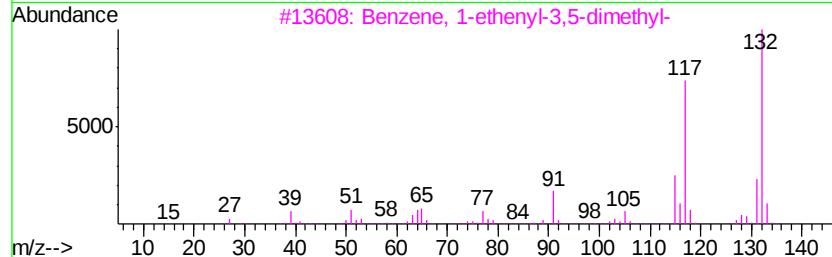
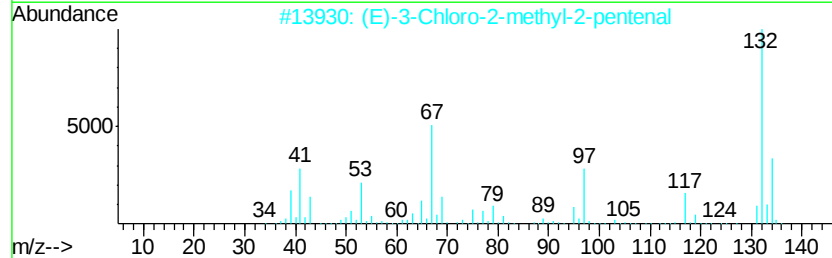
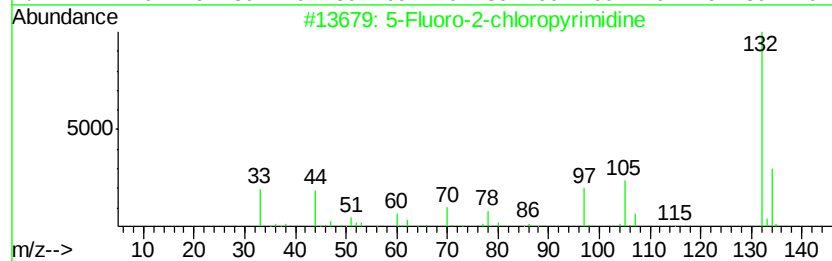
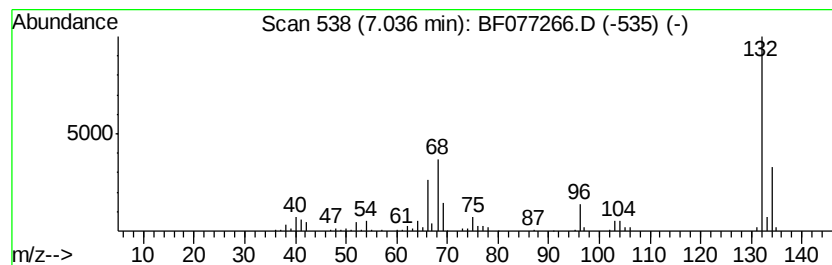
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Peak Number 3 unknown7.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.04	90.20 ng	712673	1,4-Dichlorobenzene-d4	7.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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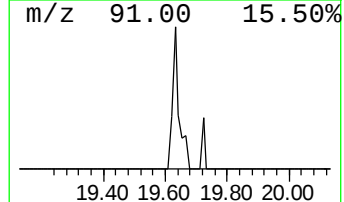
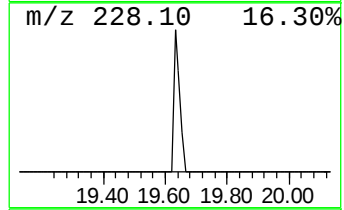
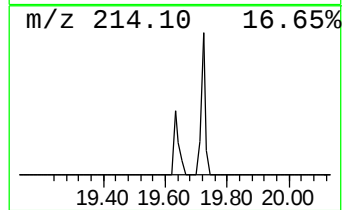
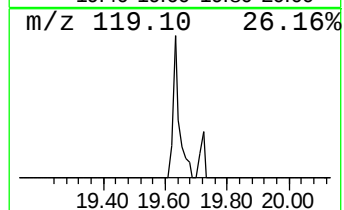
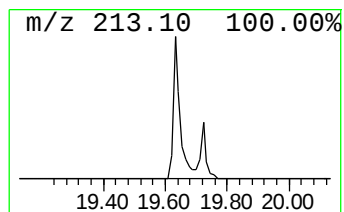
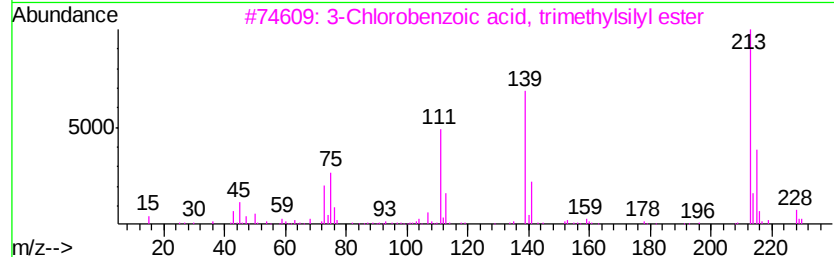
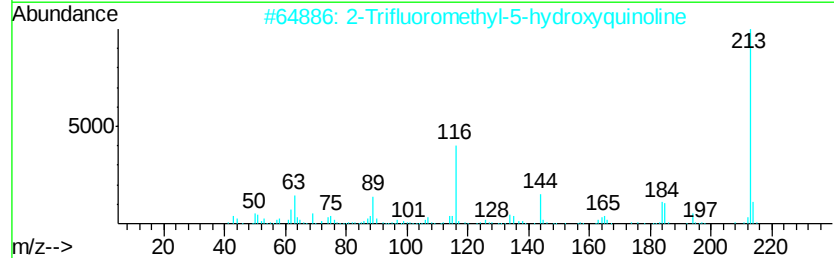
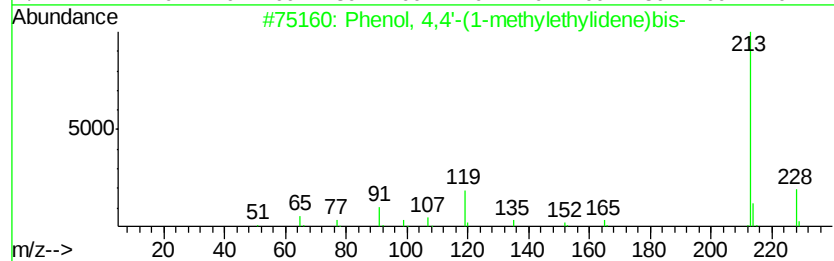
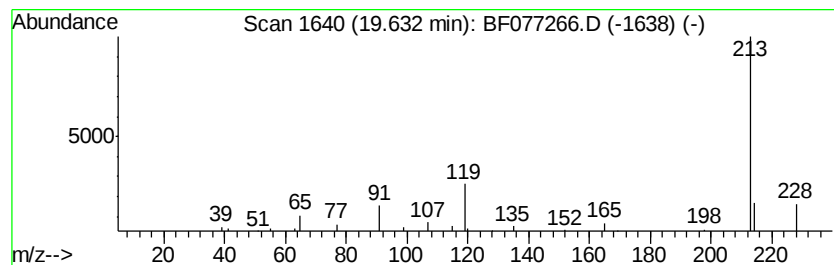
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Peak Number 6 Phenol, 4,4'-(1-methylethyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
19.63	2.50 ng	38160	Chrysene-d12	20.98		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	91	
2	2-Trifluoromethyl-5-hydroxyquino...	213	C10H6F3NO	041958-06-9	53	
3	3-Chlorobenzoic acid, trimethyls...	228	C10H13ClO2Si	114521-53-8	42	
4	Pyridine, 3-(5-trifluoromethyl-3...	213	C9H6F3N3	003974-70-7	40	
5	Carbamic acid, [1,1'-biphenyl]-3...	213	C13H11NO2	055030-29-0	38	



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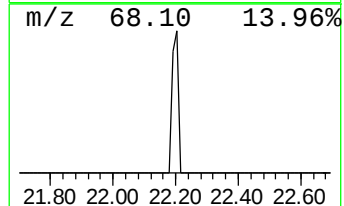
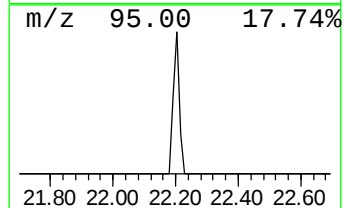
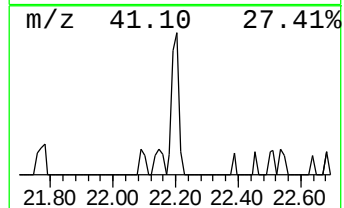
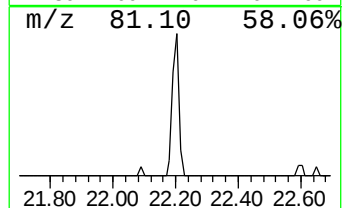
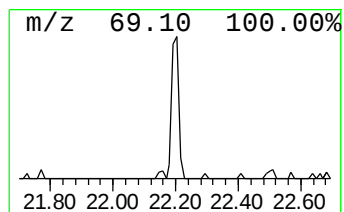
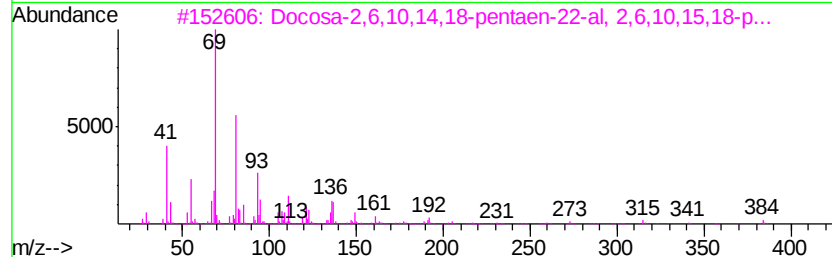
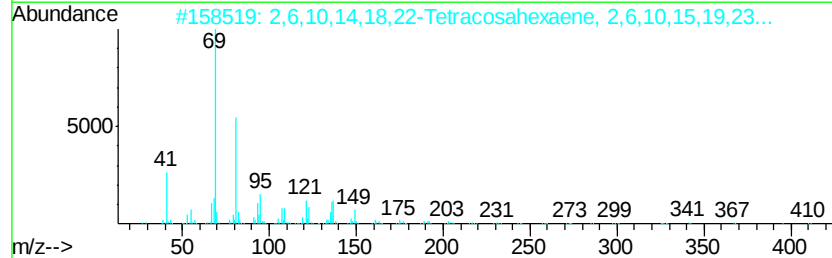
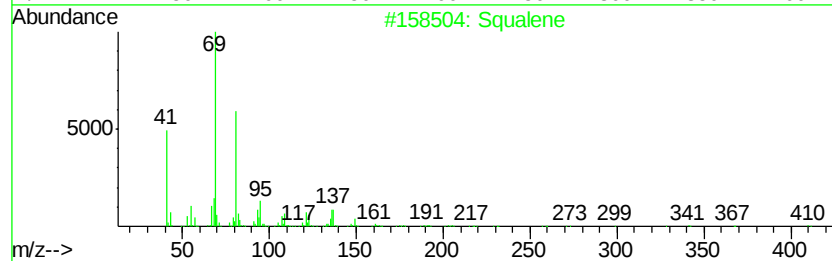
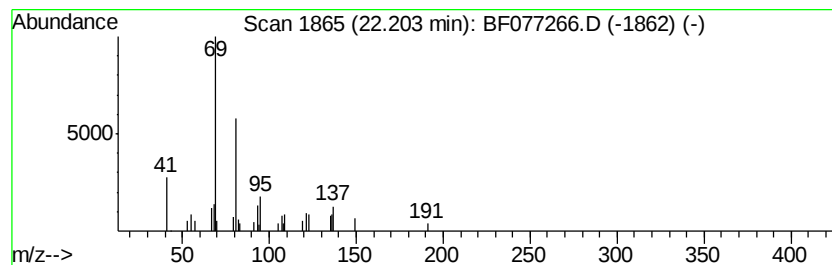
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Peak Number 7 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.20	3.41 ng	41599	Perylene-d12	22.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	90
2		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	90
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	86
4		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72
5		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	3.54	23.4	ng	184699	1	7.54	158021	20.0
unknown7.04	7.04	90.2	ng	712673	1	7.54	158021	20.0
Phenol, 4,4'-(1-m...	19.63	2.5	ng	38160	5	20.98	305174	20.0
Squalene	22.20	3.4	ng	41599	6	22.61	244257	20.0