

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF071618\
 Data File : BF107433.D
 Acq On : 17 Jul 2018 5:13
 Operator : JU/SJ
 Sample : J3633-01
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A-1(0-6)

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.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	5.219	486	490	498	rVB	351896	420108	13.35%	1.496%
2	5.613	552	557	560	rBV	3243975	3032252	96.38%	10.794%
3	6.607	720	726	729	rBV	3163819	3146179	100.00%	11.200%
4	6.754	746	751	754	rBV	3409198	3093126	98.31%	11.011%
5	6.913	772	778	780	rVB5	22217	34402	1.09%	0.122%
6	6.983	786	790	794	rVB	1190080	930173	29.57%	3.311%
7	7.142	813	817	820	rVB	2650493	2320307	73.75%	8.260%
8	7.548	881	886	889	rBV	1943434	1859793	59.11%	6.620%
9	8.266	1004	1008	1012	rBV	1161254	993364	31.57%	3.536%
10	9.342	1186	1191	1194	rBV	3207526	2750950	87.44%	9.793%
11	9.442	1204	1208	1211	rBV3	28809	34280	1.09%	0.122%
12	9.730	1254	1257	1261	rBV	491826	395424	12.57%	1.408%
13	10.030	1301	1308	1311	rBV	1100095	1027112	32.65%	3.656%
14	10.819	1438	1442	1445	rBV	2064207	1787152	56.80%	6.362%
15	11.518	1557	1561	1564	rBV	1227633	1092894	34.74%	3.890%
16	11.966	1634	1637	1640	rVB4	40388	42029	1.34%	0.150%
17	12.383	1705	1708	1710	rBV4	35557	42526	1.35%	0.151%
18	12.542	1732	1735	1737	rVB4	50025	45910	1.46%	0.163%
19	12.748	1768	1770	1773	rBV4	30490	34226	1.09%	0.122%
20	12.989	1809	1811	1813	rVB3	43291	32624	1.04%	0.116%
21	13.107	1827	1831	1834	rBV	3172564	2886654	91.75%	10.276%
22	13.983	1978	1980	1985	rBV4	231480	252802	8.04%	0.900%
23	14.171	2008	2012	2015	rBV	1080317	1006481	31.99%	3.583%
24	15.024	2155	2157	2160	rBV3	138876	132413	4.21%	0.471%
25	15.706	2269	2273	2278	rBV	493975	698287	22.19%	2.486%

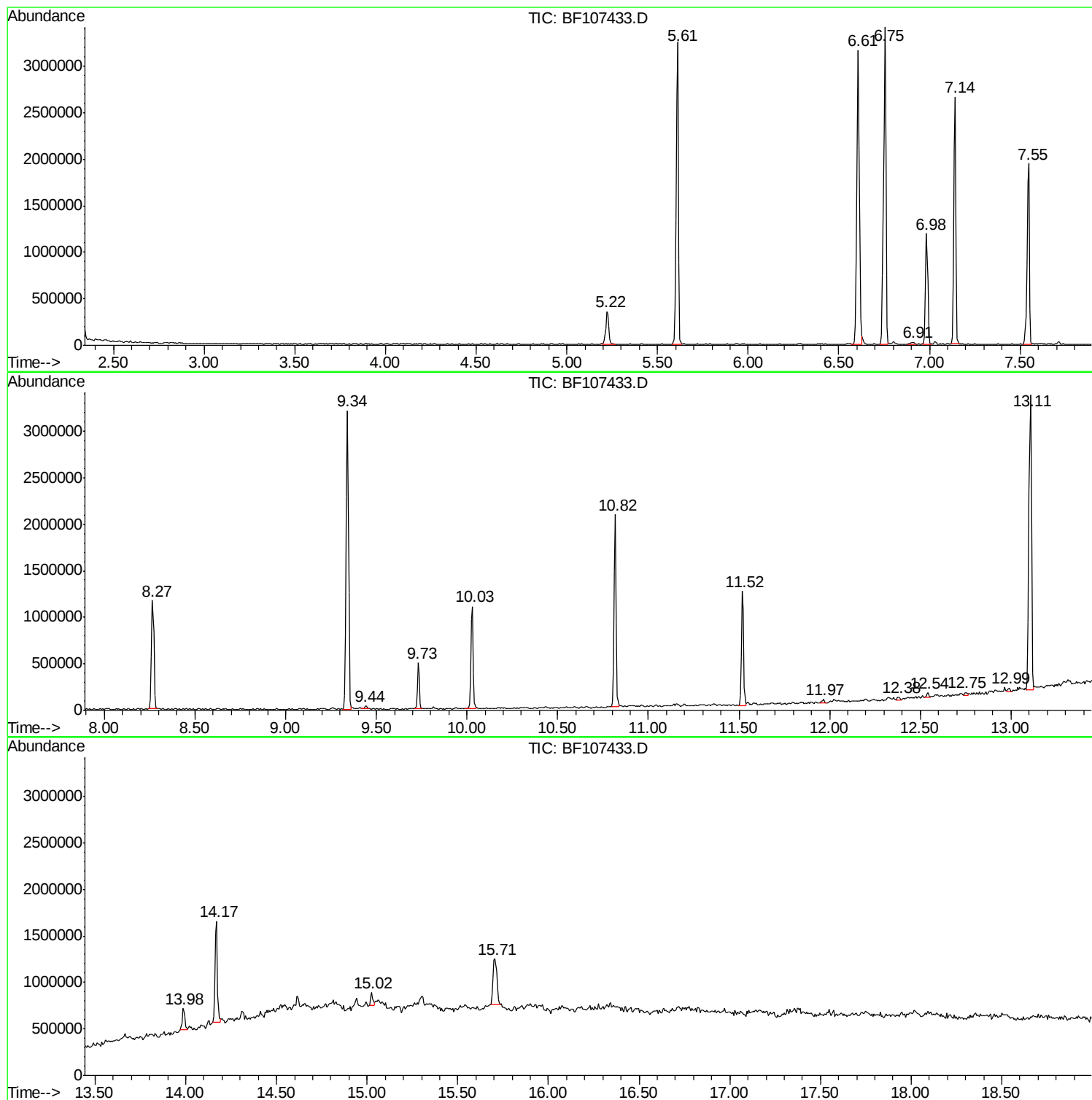
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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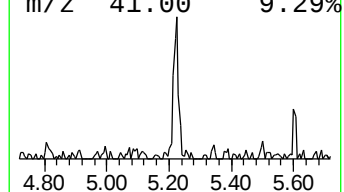
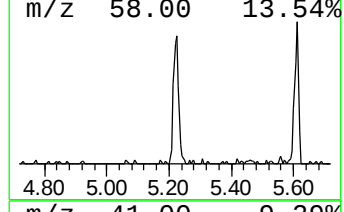
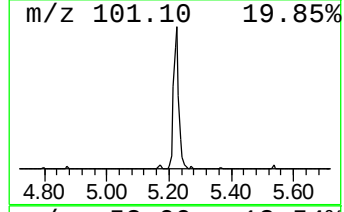
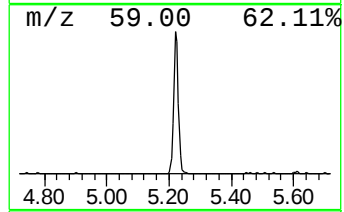
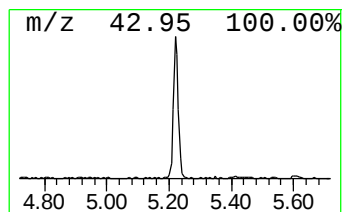
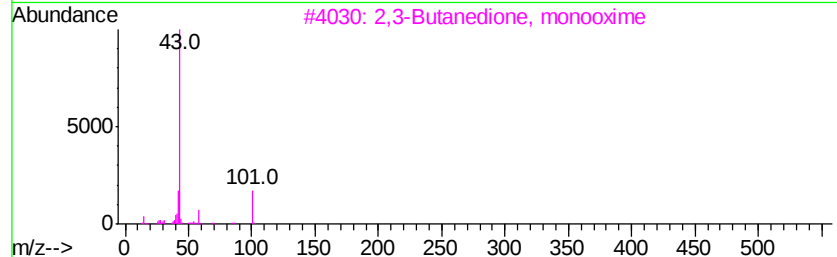
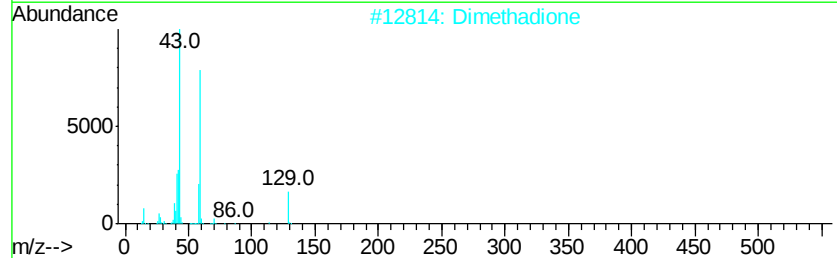
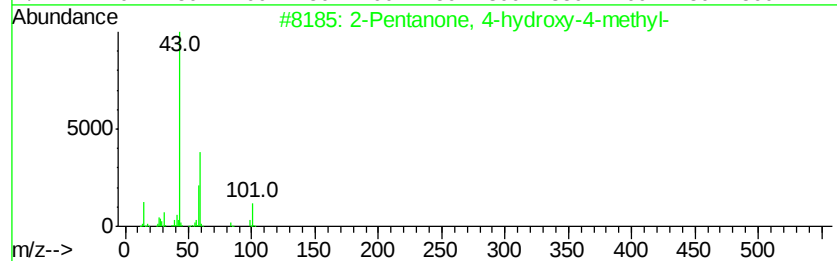
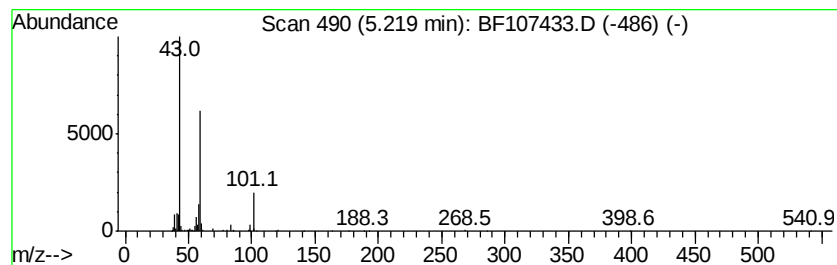
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	3.62 ng	420108	1,4-Dichlorobenzene-d4	7.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39	
2	Dimethadione	129	C5H7NO3	000695-53-4	36	
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25	
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25	
5	Methyl 2,5,8,11-tetraoxatridecan...	236	C10H20O6	1000366-78-2	23	



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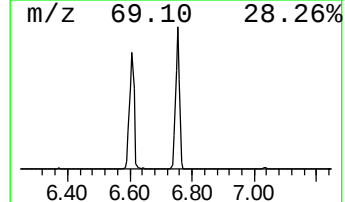
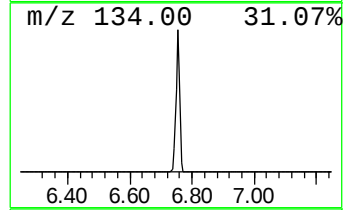
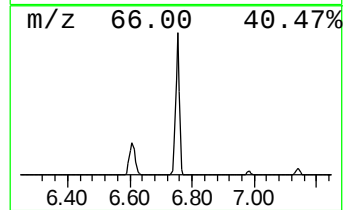
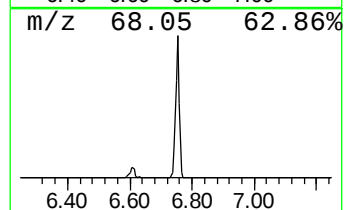
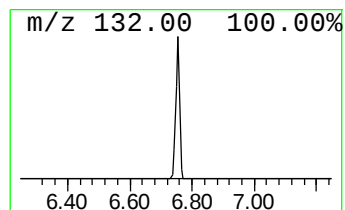
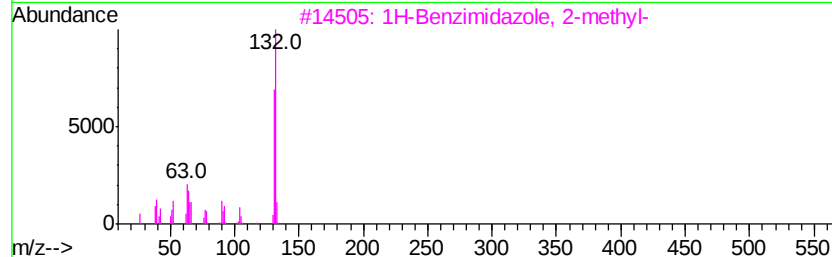
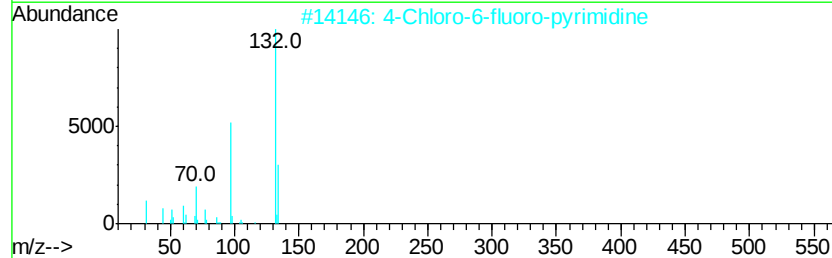
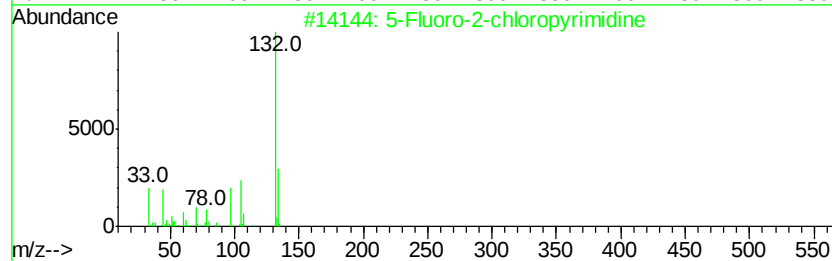
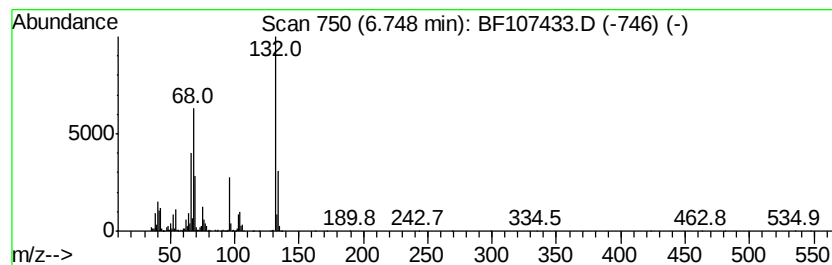
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Peak Number 2 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	26.66 ng	3093130	1,4-Dichlorobenzene-d4	7.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	10



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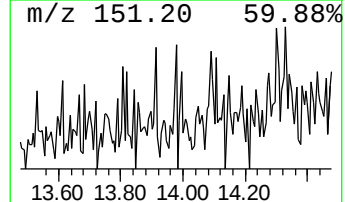
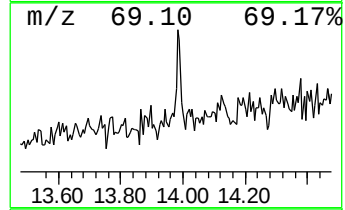
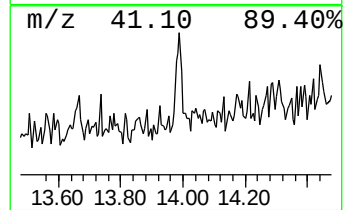
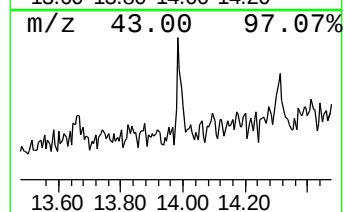
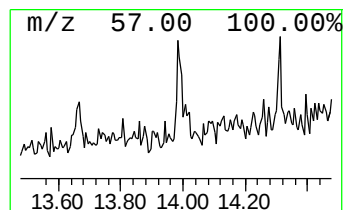
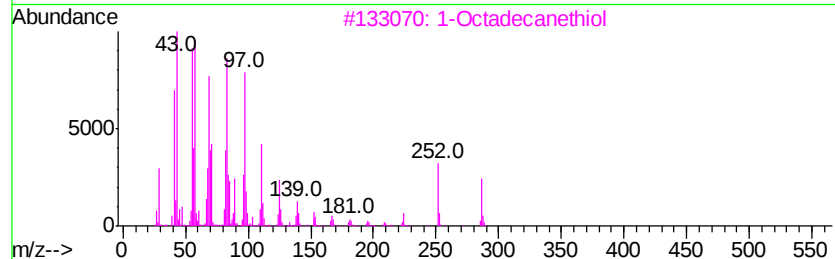
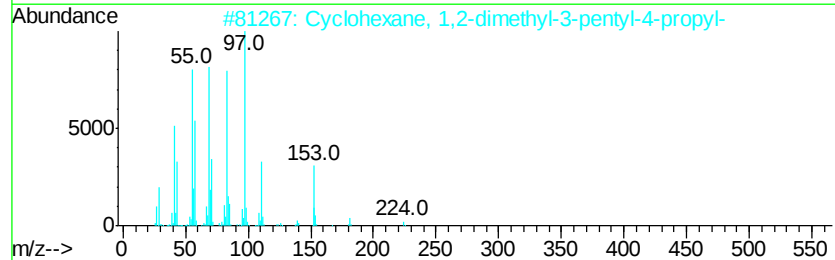
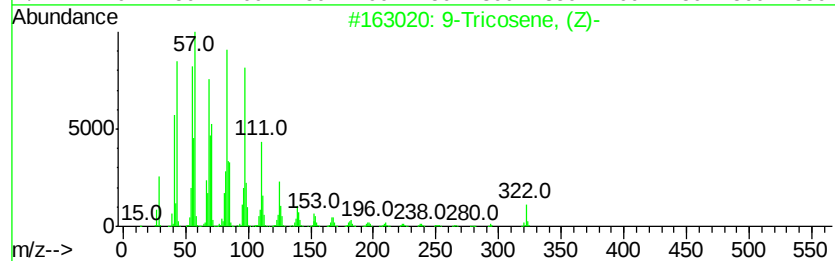
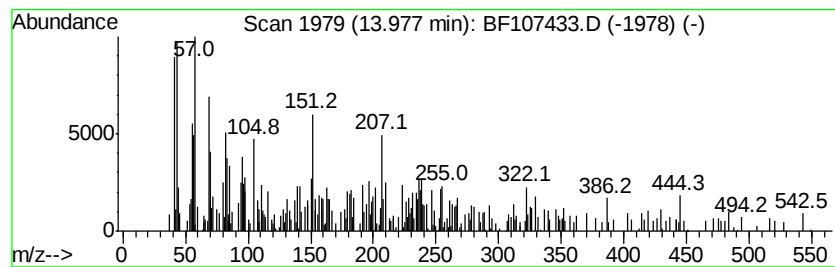
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Peak Number 4 9-Tricosene, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.98	5.02 ng	252802	Chrysene-d12	14.17

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Tricosene, (Z)-	322	C23H46	027519-02-4	91
2		Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	91
3		1-Octadecanethiol	286	C18H38S	002885-00-9	91
4		9-Hexacosene	364	C26H52	071502-22-2	91
5		4-Methyl-E-9-octadecene	266	C19H38	1000130-87-1	91



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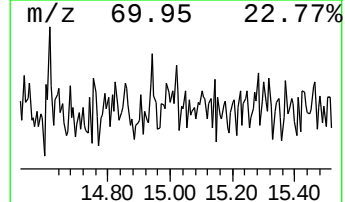
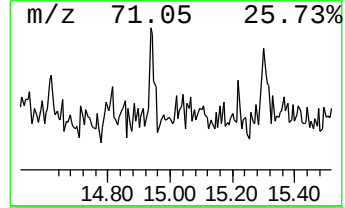
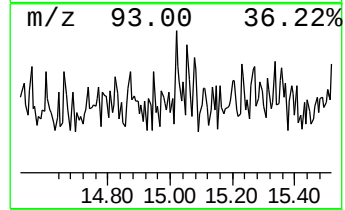
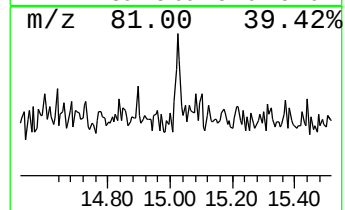
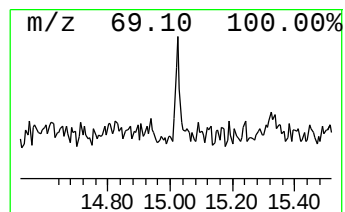
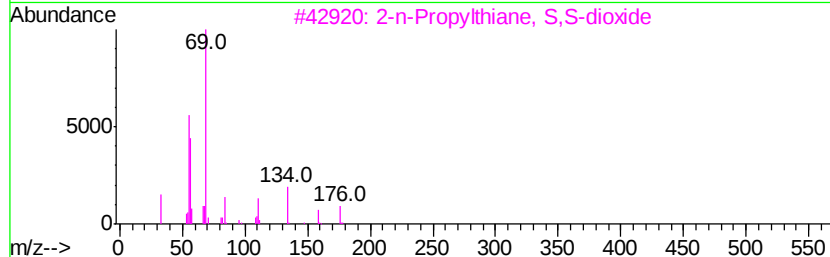
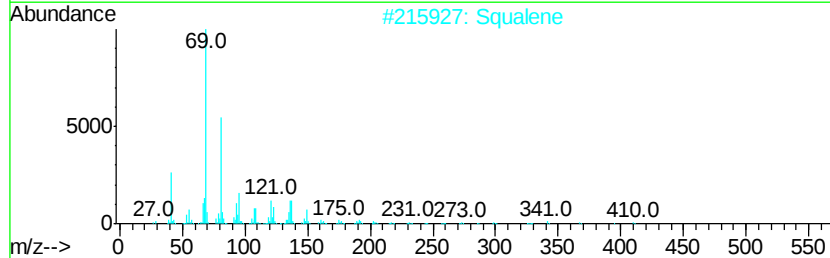
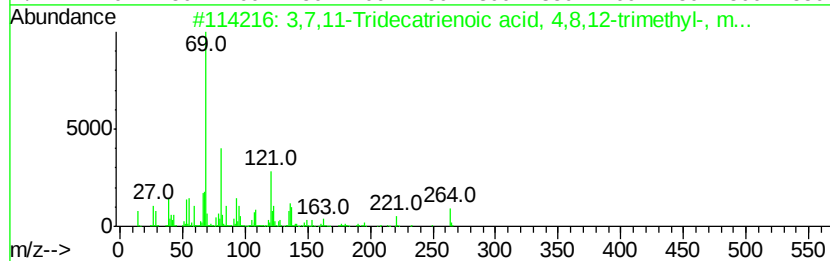
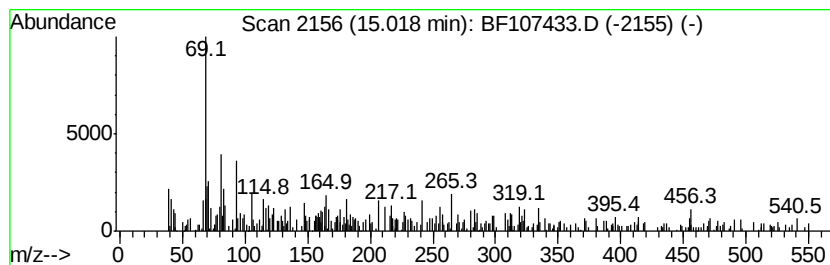
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Peak Number 5 3,7,11-Tridecatrienoic acid... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	3.79 ng	132413	Perylene-d12	15.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,7,11-Tridecatrienoic acid, 4,8...	264	C17H28O2	036237-70-4	58
2		Squalene	410	C30H50	000111-02-4	53
3		2-n-Propylthiane, S,S-dioxide	176	C8H16O2S	072385-41-2	53
4		Cyclohexanepropanal, 2,2-dimethy...	180	C12H20O	076337-22-9	53
5		2,2'-Bi-1,3,2-dioxaphosphorinane...	298	C10H20O6P2	016368-06-2	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.22	3.6	ng	420108	1	7.14	2320310	20.0
unknown6.75	6.75	26.7	ng	3093130	1	7.14	2320310	20.0
9-Tricosene, (Z)-	13.98	5.0	ng	252802	5	14.17	1006480	20.0
3,7,11-Tridecatri...	15.02	3.8	ng	132413	6	15.71	698287	20.0