

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080818\
 Data File : BM016252.D
 Acq On : 08 Aug 2018 16:28
 Operator : SJ/JU
 Sample : J4283-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TR-04-080318

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_M\METHODS\8270-BM072318.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	5.187	318	323	335	rVB	97111	146854	8.17%	1.147%
2	5.663	398	404	421	rBV	655457	1008309	56.08%	7.879%
3	7.304	677	683	700	rBV	620664	1048270	58.30%	8.191%
4	7.663	738	744	755	rBV	729997	1152907	64.12%	9.009%
5	8.134	819	824	835	rBB	206526	333170	18.53%	2.603%
6	8.457	872	879	890	rBB	531016	857492	47.69%	6.700%
7	9.322	1020	1026	1043	rBV	380571	640963	35.65%	5.008%
8	10.951	1297	1303	1314	rBV	234513	389569	21.67%	3.044%
9	13.392	1711	1718	1729	rBV	823888	1202276	66.87%	9.394%
10	14.222	1853	1859	1868	rVB	66045	90944	5.06%	0.711%
11	14.769	1945	1952	1959	rBV2	301678	454341	25.27%	3.550%
12	16.257	2199	2205	2216	rBV	751877	1050824	58.45%	8.211%
13	17.504	2412	2417	2423	rBV	366831	520557	28.95%	4.068%
14	17.551	2423	2425	2430	rVB	19539	20566	1.14%	0.161%
15	18.357	2556	2562	2570	rBV3	109954	168713	9.38%	1.318%
16	18.427	2570	2574	2579	rVB5	9421	18519	1.03%	0.145%
17	18.568	2593	2598	2602	rBV6	13449	25263	1.41%	0.197%
18	19.262	2712	2716	2717	rBV2	19926	25298	1.41%	0.198%
19	19.286	2717	2720	2723	rVB3	25653	32773	1.82%	0.256%
20	19.539	2759	2763	2769	rVB	65505	92199	5.13%	0.720%
21	19.615	2772	2776	2783	rVV3	51862	72361	4.02%	0.565%
22	19.904	2821	2825	2831	rVB	90754	125432	6.98%	0.980%
23	20.086	2851	2856	2861	rBV	1529433	1797963	100.00%	14.049%
24	20.356	2898	2902	2904	rBV5	21319	27416	1.52%	0.214%
25	21.303	3061	3063	3070	rVB3	76269	108328	6.03%	0.846%
26	21.639	3114	3120	3124	rBV	512084	726021	40.38%	5.673%
27	23.974	3512	3517	3524	rVB	356105	660483	36.74%	5.161%

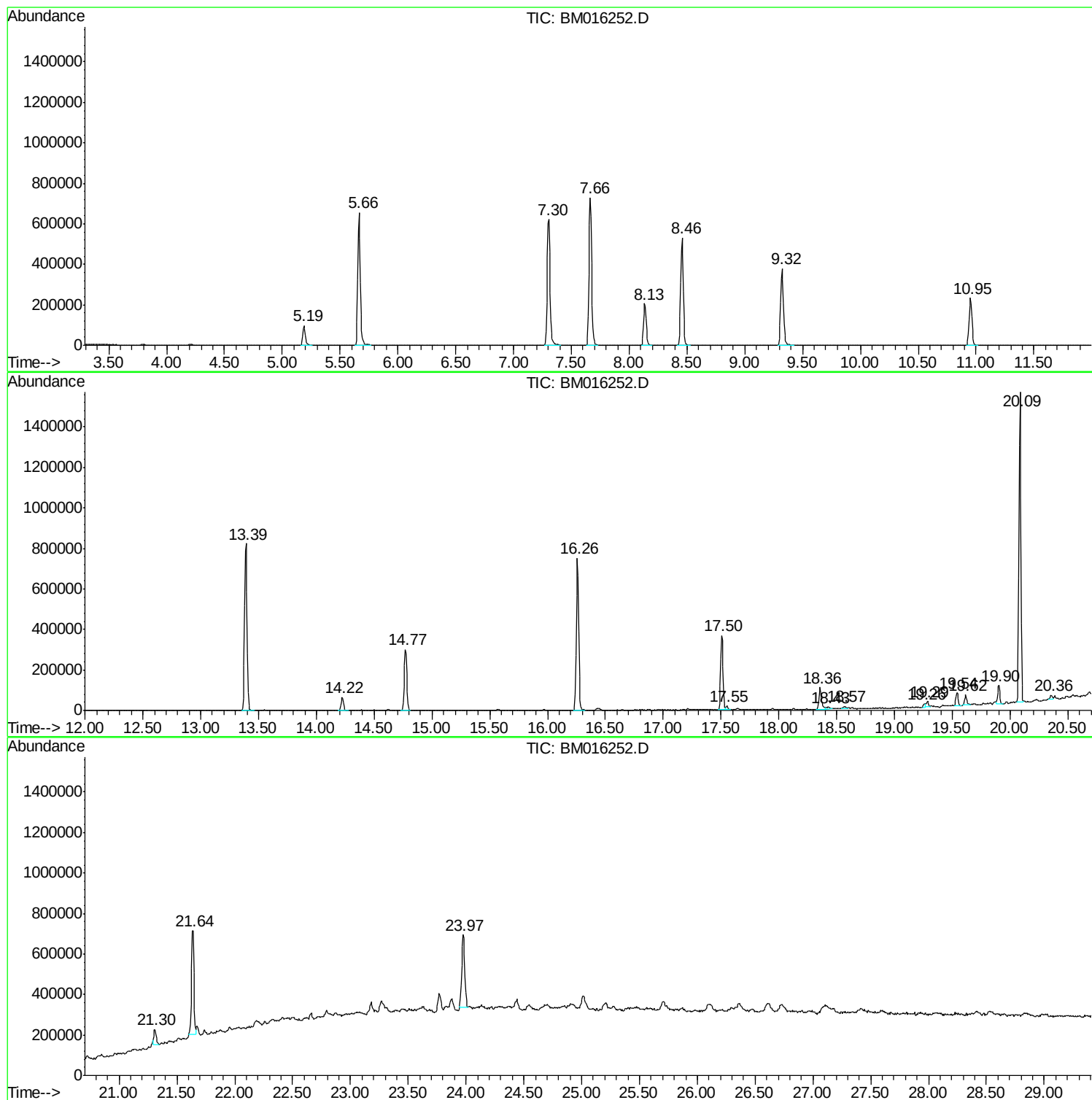
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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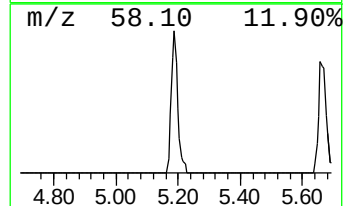
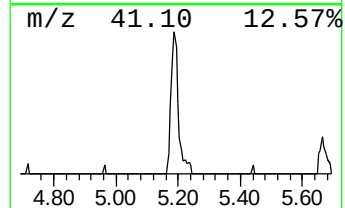
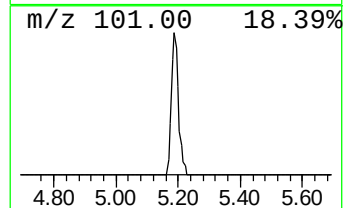
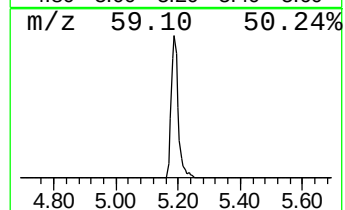
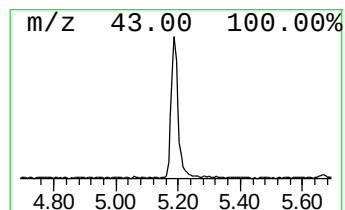
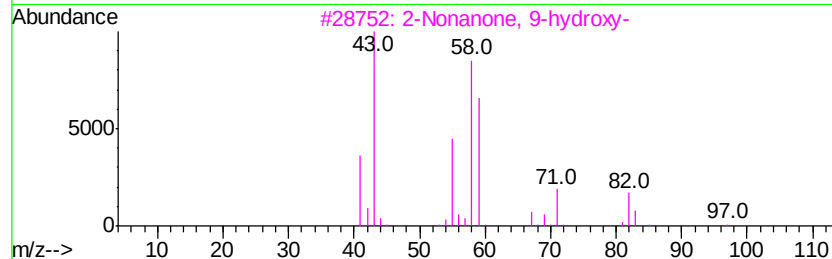
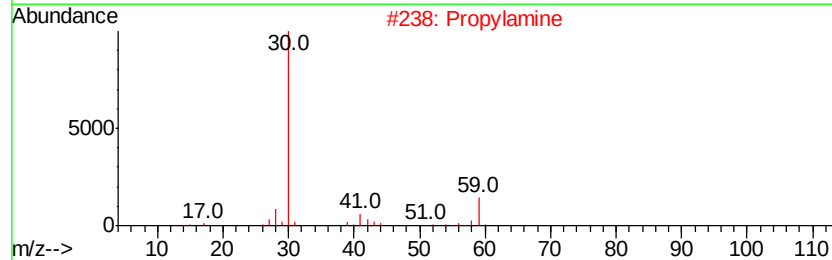
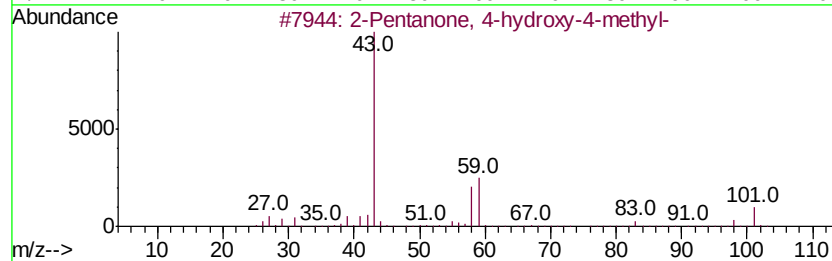
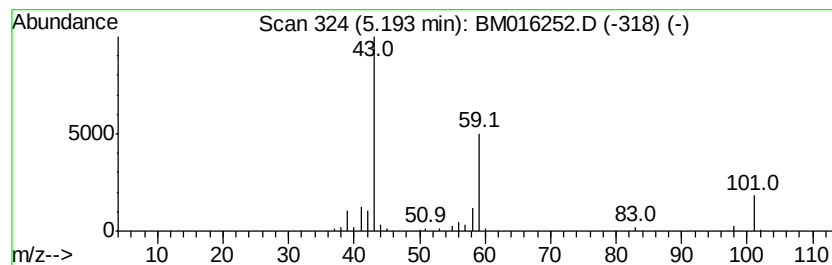
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	8.82 ng	146854	1,4-Dichlorobenzene-d4	8.13

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propylamine	59	C3H9N	000107-10-8	40
3			2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	36
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5			Butane	58	C4H10	000106-97-8	12



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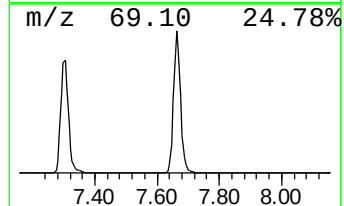
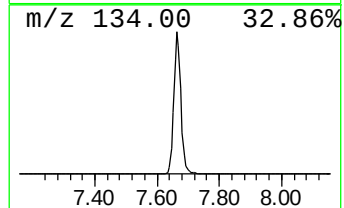
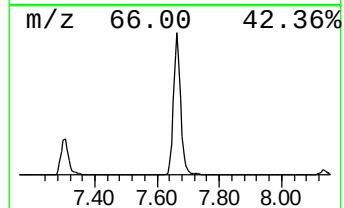
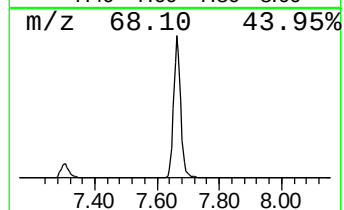
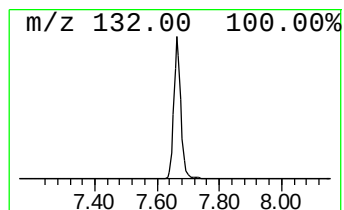
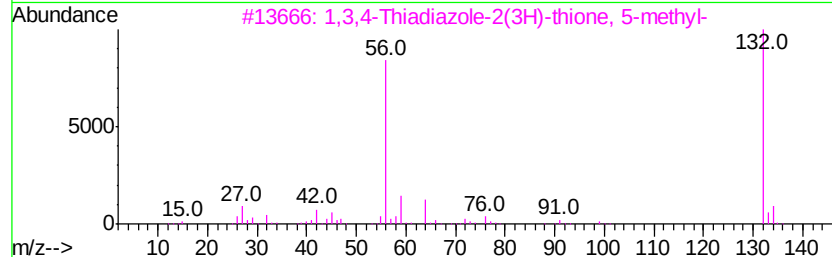
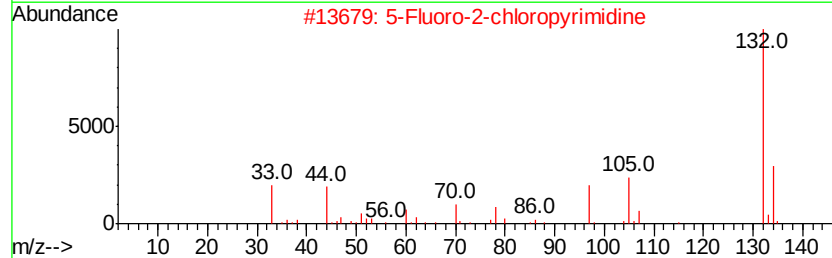
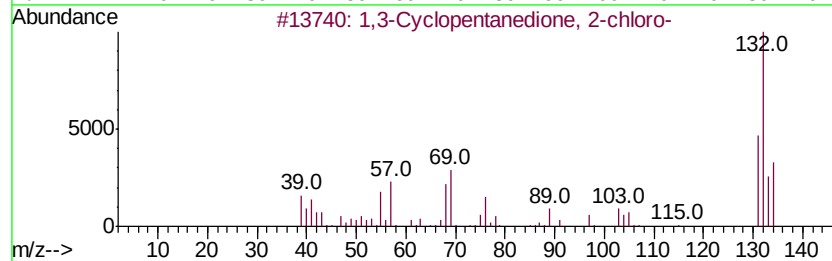
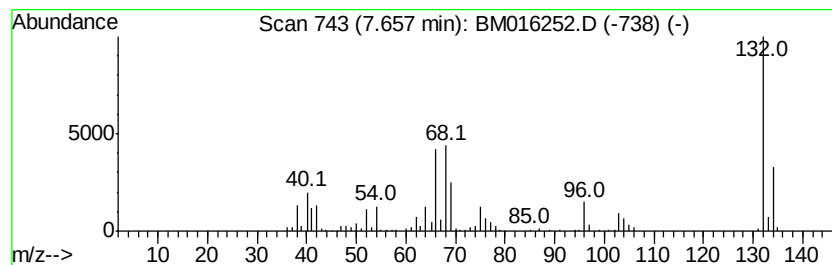
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Peak Number 2 unknown7.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	69.21 ng	1152910	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	16
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
3		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
4		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
5		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10



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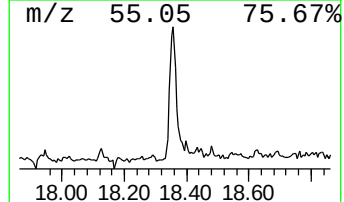
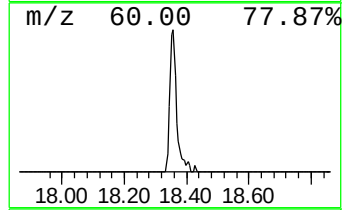
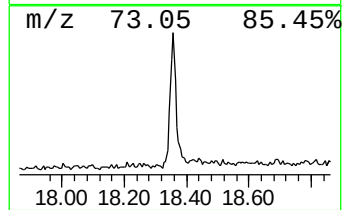
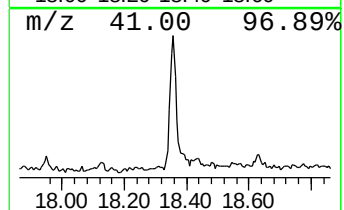
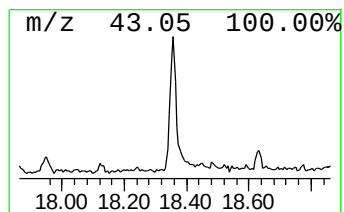
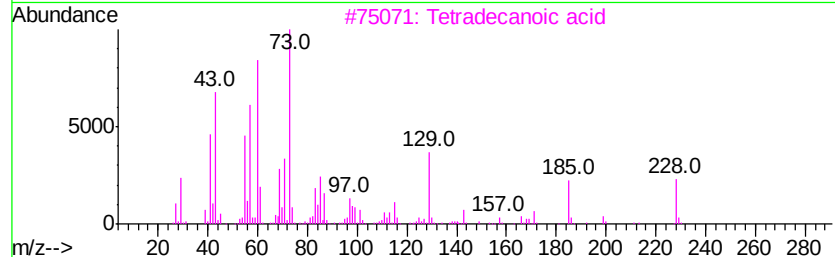
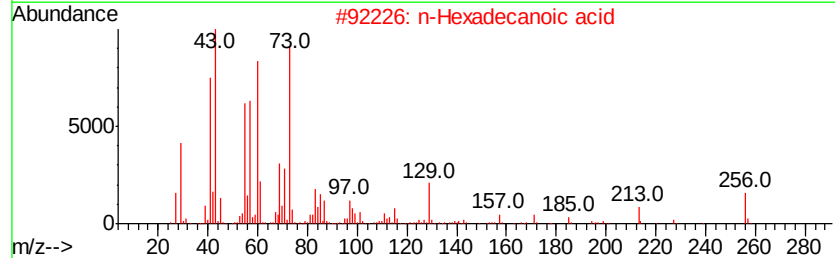
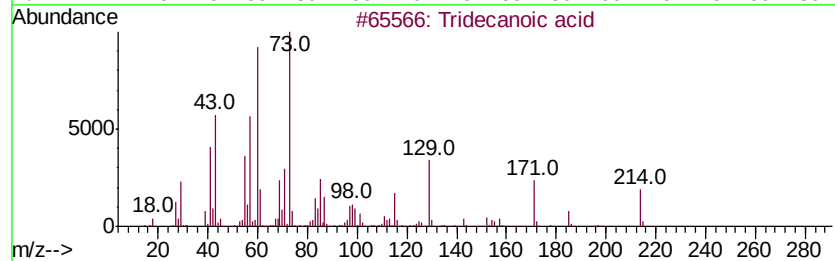
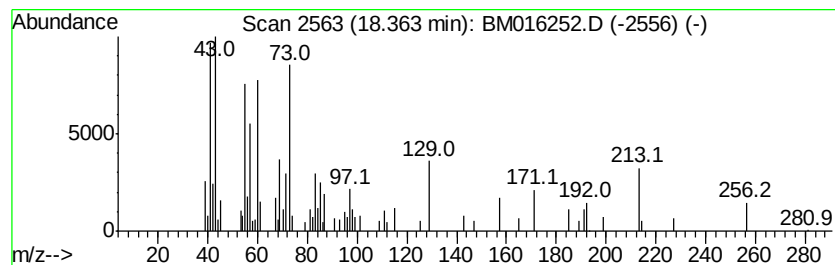
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Peak Number 4 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.36	6.48 ng	168713	Phenanthrene-d10		17.50
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	76
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4	n-Decanoic acid	172	C10H20O2	000334-48-5	46
5	Nonanoic acid	158	C9H18O2	000112-05-0	43



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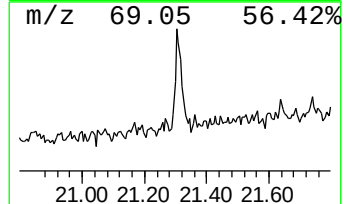
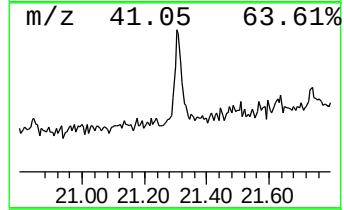
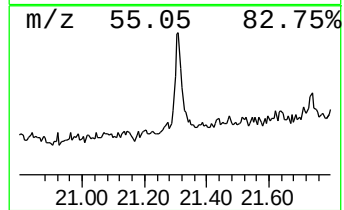
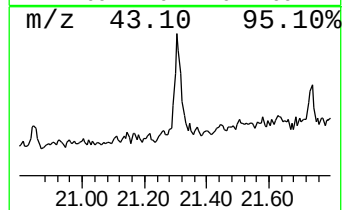
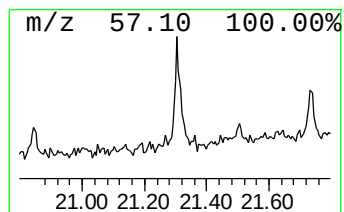
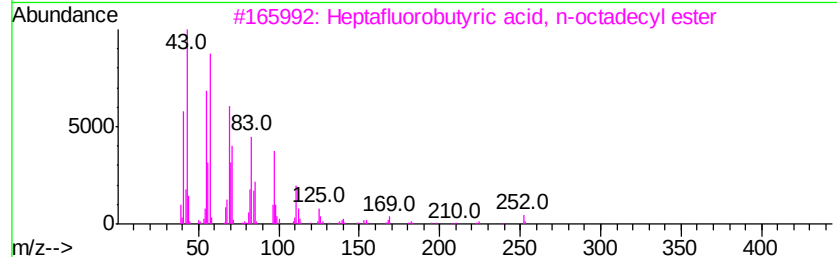
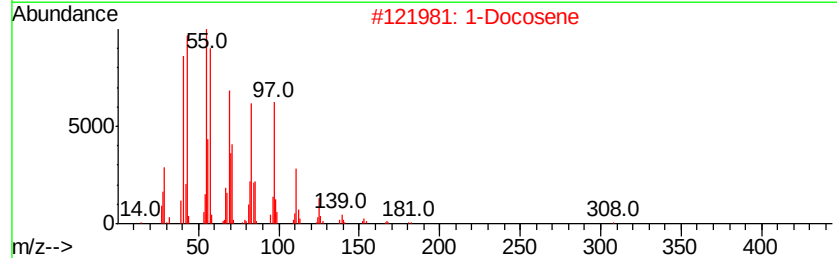
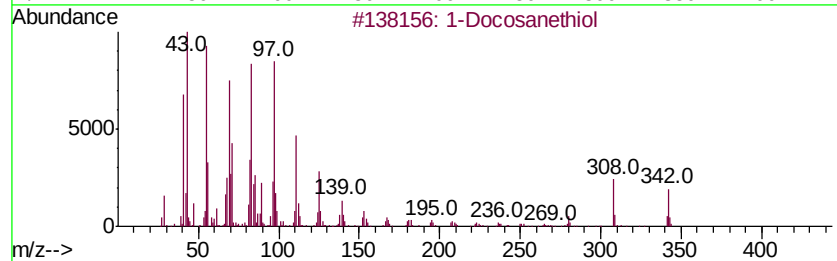
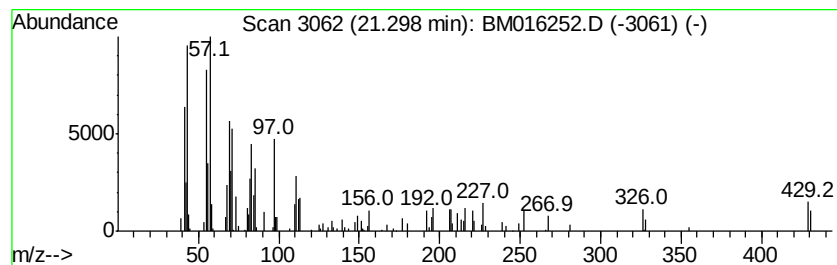
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Peak Number 5 1-Docosanethiol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.30	2.98 ng	108328	Chrysene-d12	21.64
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Docosanethiol	342 C22H46S	007773-83-3	91
2	1-Docosene	308 C22H44	001599-67-3	83
3	Heptafluorobutyric acid, n-octad...	466 C22H37F7O2	000400-57-7	81
4	1-Heptacosanol	396 C27H56O	002004-39-9	80
5	Heptafluorobutyric acid, n-penta...	424 C19H31F7O2	1000216-79-3	68



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.19	8.8	ng	146854	1	8.13	333170	20.0
unknown7.66	7.66	69.2	ng	1152910	1	8.13	333170	20.0
Tridecanoic acid	18.36	6.5	ng	168713	4	17.50	520557	20.0
1-Docosanethiol	21.30	3.0	ng	108328	5	21.64	726021	20.0