

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081518\
 Data File : BM016386.D
 Acq On : 15 Aug 2018 18:36
 Operator : SJ/JU
 Sample : J4471-25
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 BED-ROCK

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	5.169	315	320	329	rBV	61720	90144	7.26%	1.284%
2	5.646	395	401	418	rBV	359739	576787	46.45%	8.215%
3	7.281	674	679	693	rBV	360971	593812	47.82%	8.457%
4	7.640	734	740	750	rBV	420595	668299	53.82%	9.518%
5	8.110	815	820	829	rBB	97216	157611	12.69%	2.245%
6	8.434	868	875	883	rBV	328236	531504	42.80%	7.570%
7	9.298	1016	1022	1039	rBV	212065	370153	29.81%	5.272%
8	10.928	1293	1299	1311	rBB	105247	178235	14.35%	2.538%
9	13.369	1708	1714	1727	rBV	519628	756559	60.93%	10.775%
10	14.204	1852	1856	1863	rBB2	16402	21463	1.73%	0.306%
11	14.745	1943	1948	1956	rVB2	128056	198931	16.02%	2.833%
12	16.239	2196	2202	2215	rBB	446515	634823	51.12%	9.041%
13	17.486	2409	2414	2423	rVB2	167873	225168	18.13%	3.207%
14	18.333	2552	2558	2565	rBV2	51468	62670	5.05%	0.893%
15	19.592	2769	2772	2780	rBV2	30744	35931	2.89%	0.512%
16	20.062	2847	2852	2858	rBV	1038714	1241759	100.00%	17.685%
17	21.292	3056	3061	3069	rBV5	35454	65651	5.29%	0.935%
18	21.621	3112	3117	3123	rBV	225766	306952	24.72%	4.372%
19	23.950	3507	3513	3522	rVB	157209	305041	24.57%	4.344%

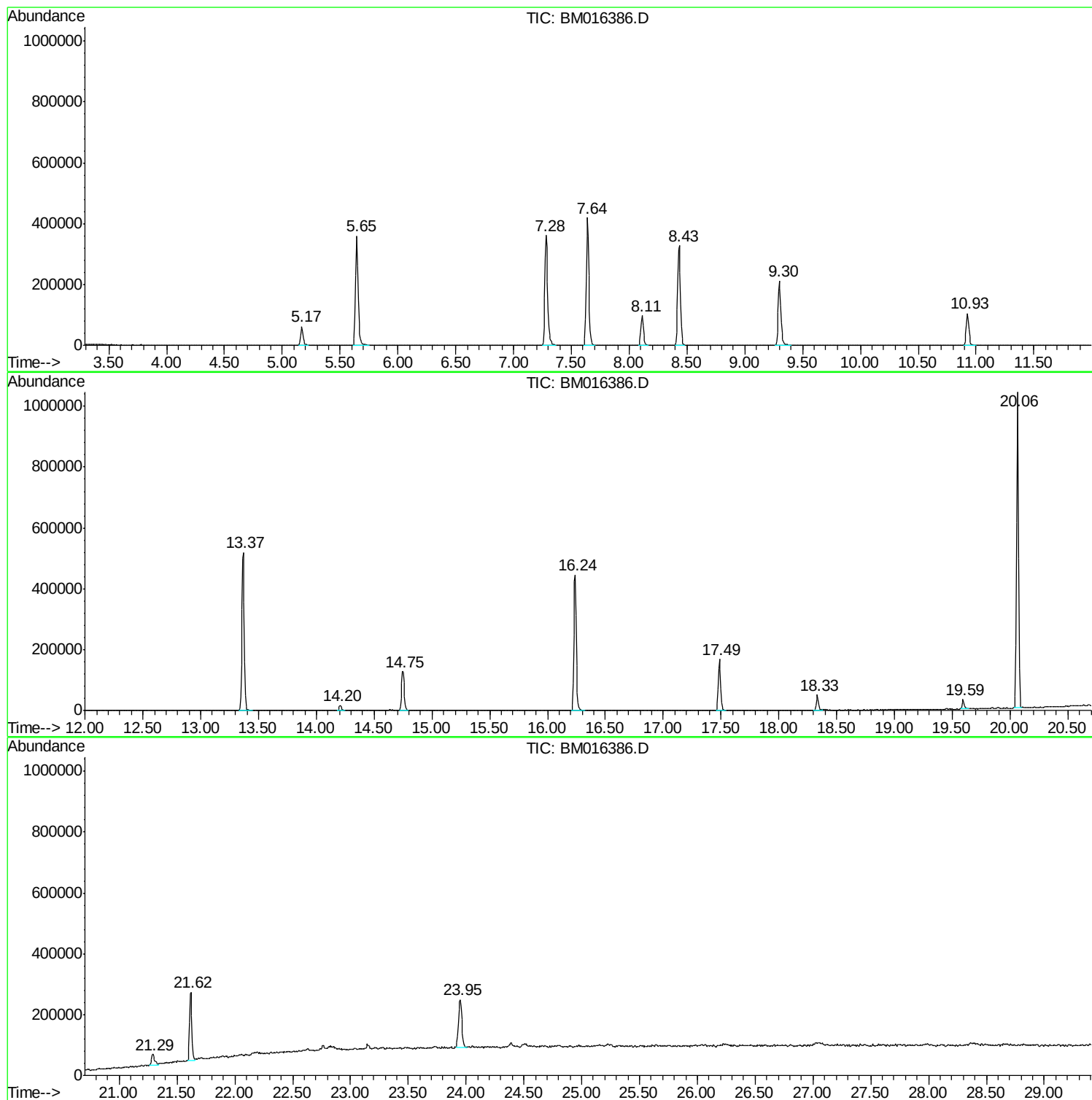
Sum of corrected areas: 7021493

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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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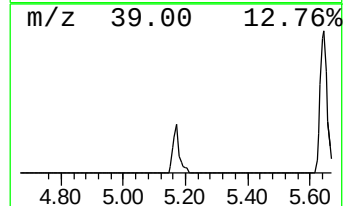
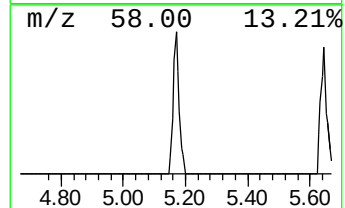
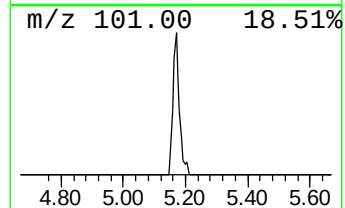
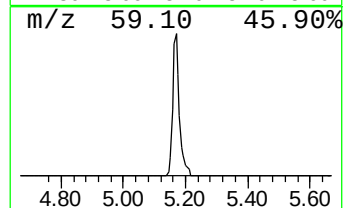
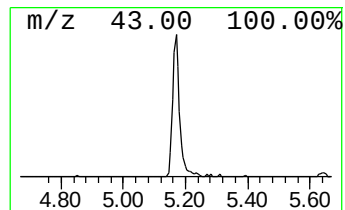
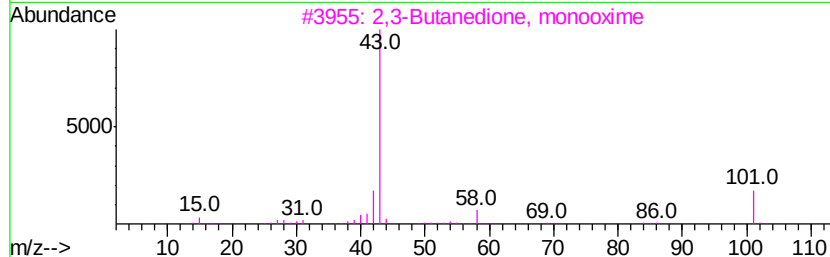
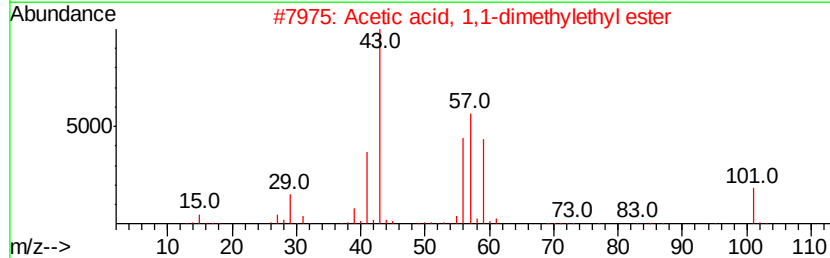
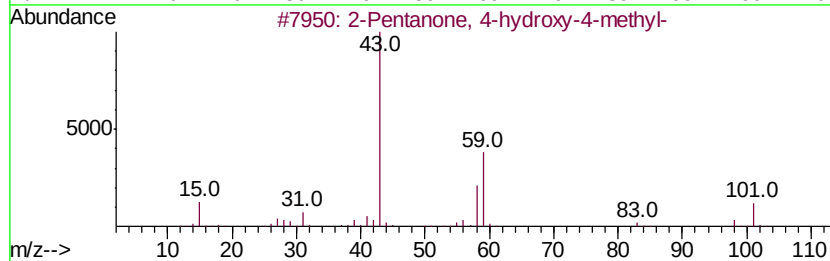
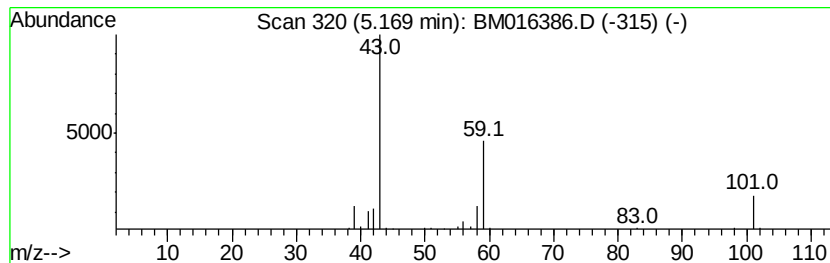
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	11.44 ng	90144	1,4-Dichlorobenzene-d4	8.11

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	36
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	16
5			Butane	58	C4H10	000106-97-8	12



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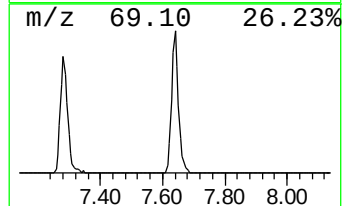
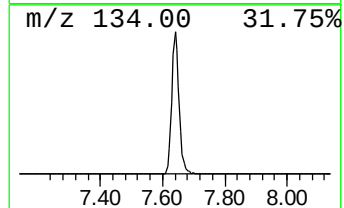
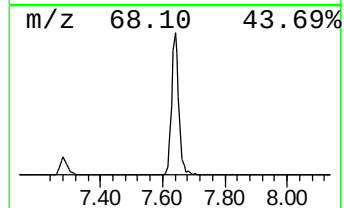
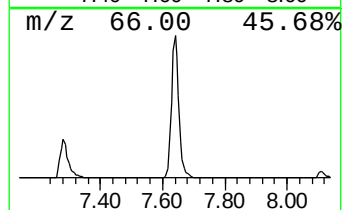
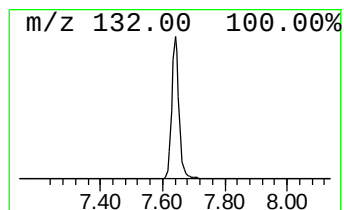
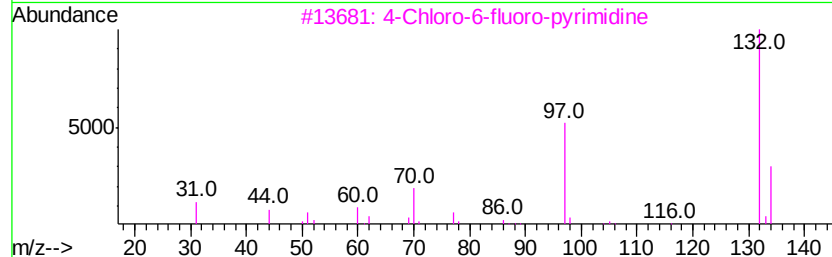
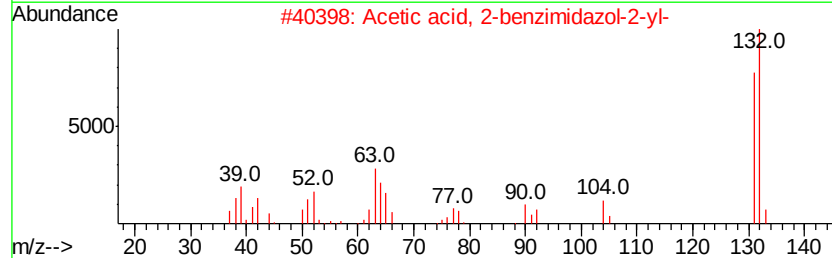
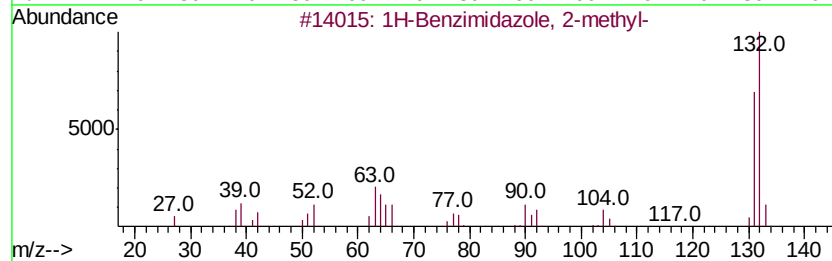
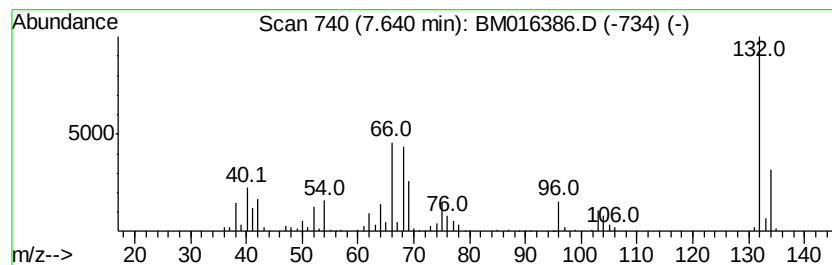
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Peak Number 2 unknown7.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	84.80 ng	668299	1,4-Dichlorobenzene-d4	8.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
2		Acetic acid, 2-benzimidazol-2-yl-	176	C9H8N2O2	013570-08-6	12
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	10
4		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	10
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	10



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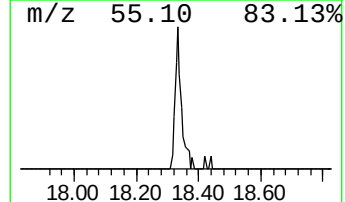
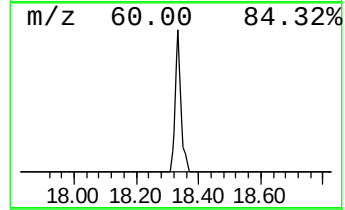
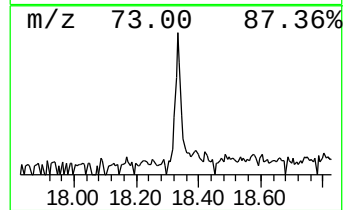
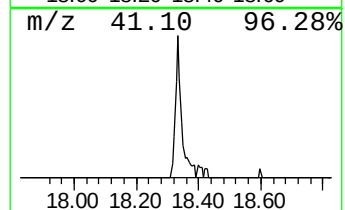
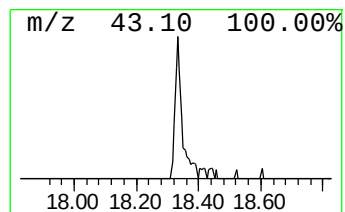
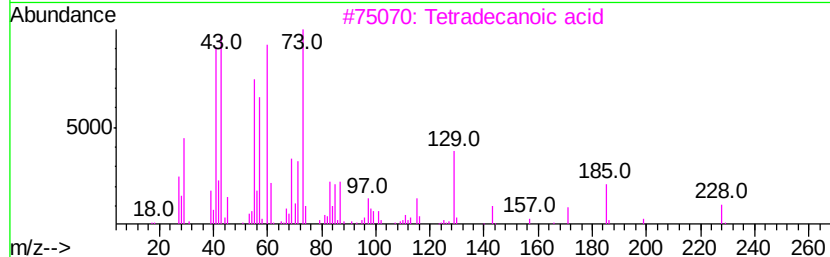
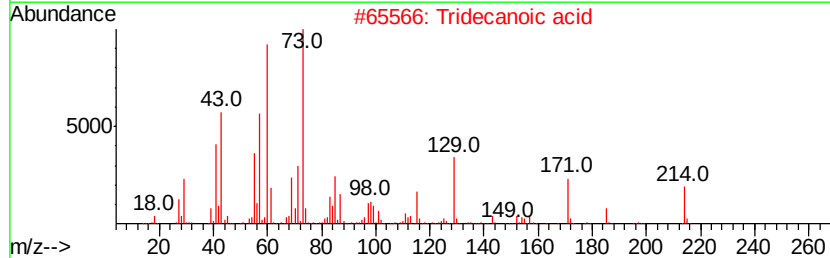
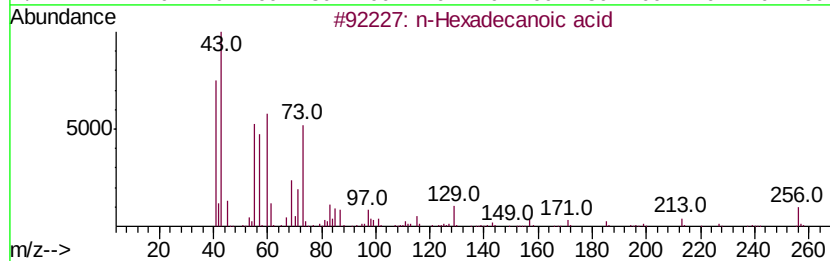
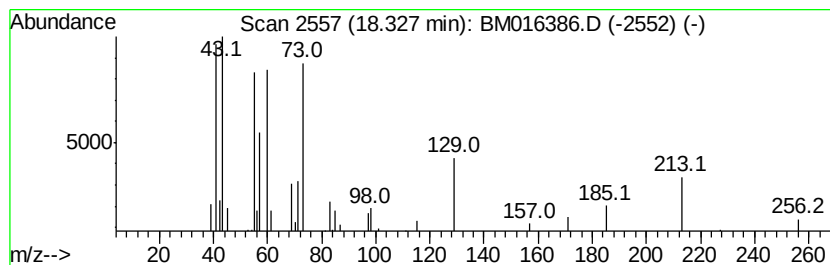
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.33	5.57 ng	62670	Phenanthrene-d10	17.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2		Tridecanoic acid	214	C13H26O2	000638-53-9	94
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4		Dodecanoic acid	200	C12H24O2	000143-07-7	50
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	47



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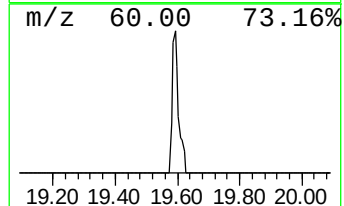
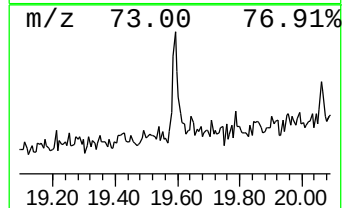
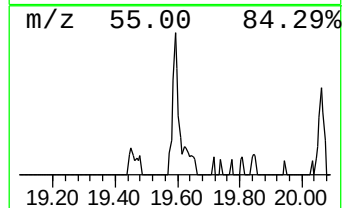
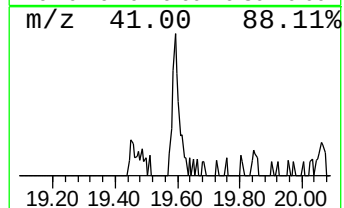
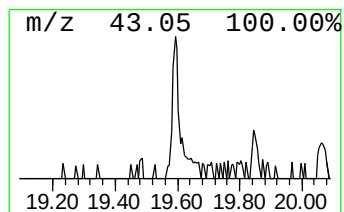
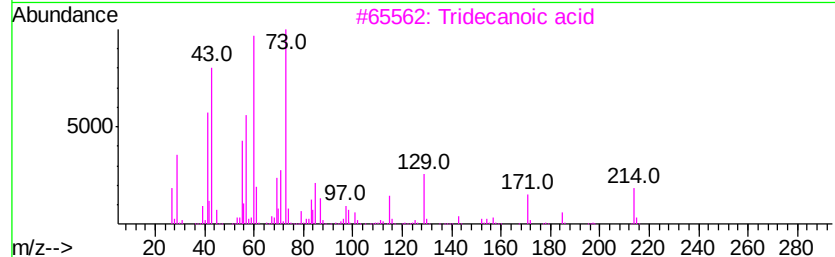
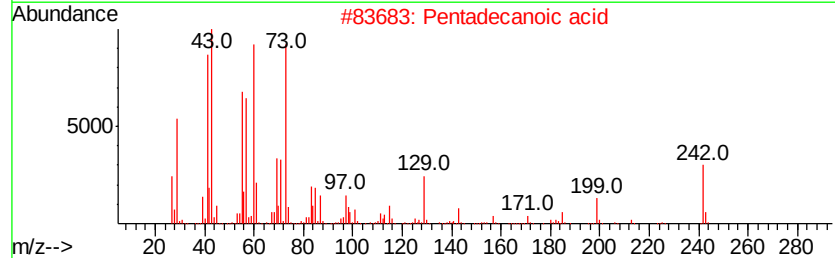
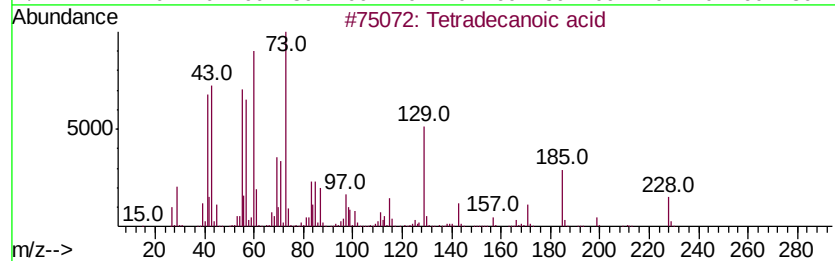
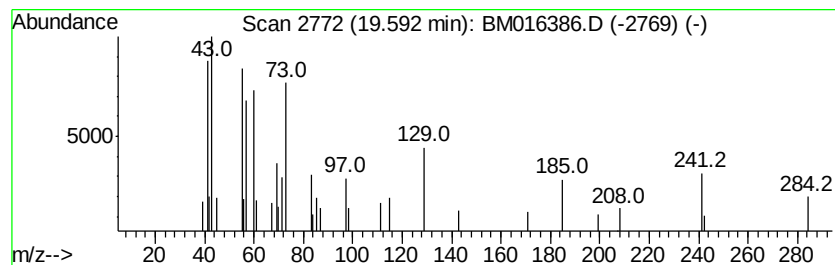
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Tetradecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.59	2.34 ng	35931	Chrysene-d12	21.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	60
3	Tridecanoic acid	214	C13H26O2	000638-53-9	43
4	n-Decanoic acid	172	C10H20O2	000334-48-5	43
5	Dodecanoic acid	200	C12H24O2	000143-07-7	43



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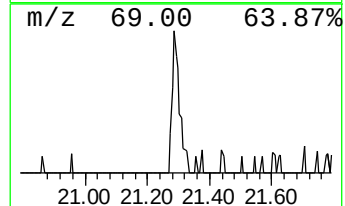
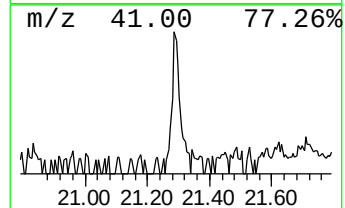
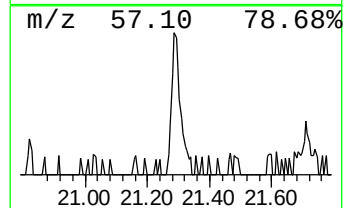
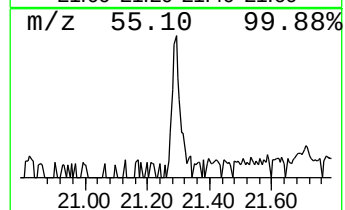
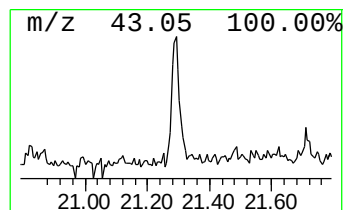
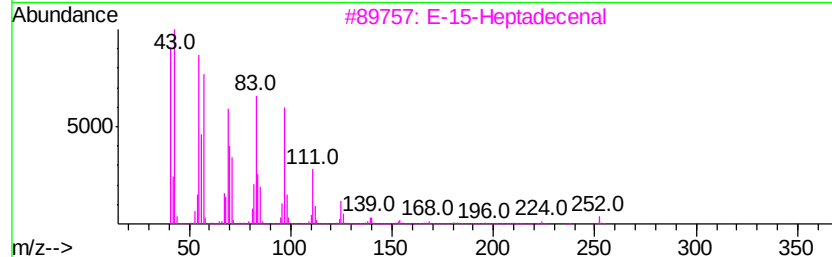
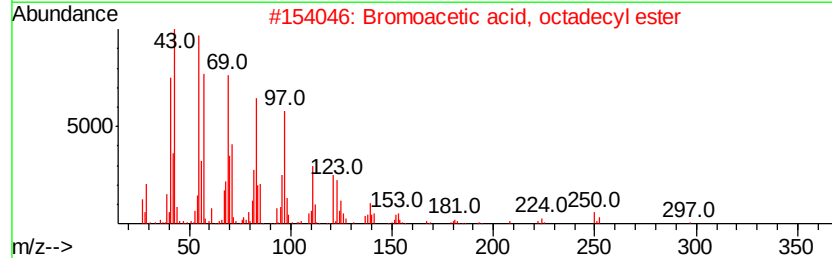
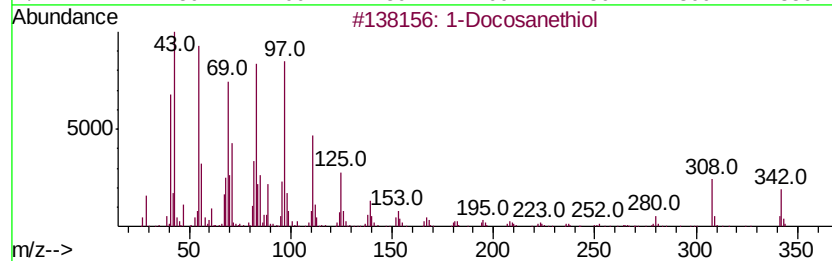
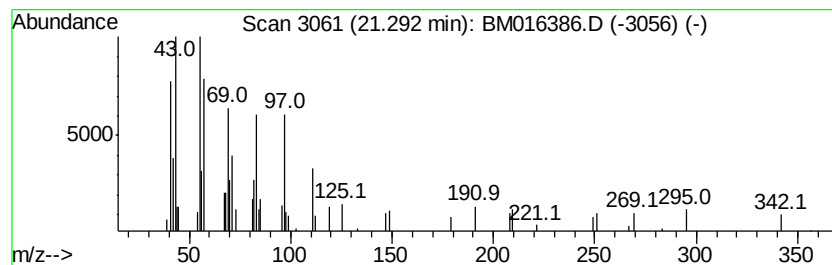
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Peak Number 6 1-Docosanethiol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.29	4.28 ng	65651	Chrysene-d12	21.62
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Docosanethiol	342 C22H46S	007773-83-3	91
2	Bromoacetic acid, octadecyl ester	390 C20H39BrO2	018992-03-5	68
3	E-15-Heptadecenal	252 C17H32O	1000130-97-9	58
4	Dichloroacetic acid, tetradecyl ...	324 C16H30Cl2O2	083005-02-1	58
5	Acetic acid, chloro-, octadecyl ...	346 C20H39ClO2	005348-82-3	49



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.17	11.4	ng	90144	1	8.11	157611	20.0
unknown7.64	7.64	84.8	ng	668299	1	8.11	157611	20.0
n-Hexadecanoic acid	18.33	5.6	ng	62670	4	17.49	225168	20.0
Tetradecanoic acid	19.59	2.3	ng	35931	5	21.62	306952	20.0
1-Docosanethiol	21.29	4.3	ng	65651	5	21.62	306952	20.0