

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
 Data File : BM016362.D
 Acq On : 14 Aug 2018 19:39
 Operator : SJ/JU
 Sample : J4431-02
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 GMW-1

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:\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	331	rBV	52239	78978	4.38%	0.819%
2	5.651	397	402	419	rBB	234235	381297	21.14%	3.954%
3	7.287	675	680	694	rBV	129466	234054	12.97%	2.427%
4	7.645	735	741	751	rBV	477499	777046	43.07%	8.057%
5	8.116	815	821	831	rVB	160006	254493	14.11%	2.639%
6	8.434	868	875	888	rVB	587246	948795	52.59%	9.838%
7	9.304	1016	1023	1035	rBV	428251	719212	39.87%	7.458%
8	10.927	1293	1299	1309	rVB	166150	276908	15.35%	2.871%
9	13.368	1708	1714	1726	rVB	958482	1354132	75.06%	14.041%
10	14.204	1851	1856	1862	rBV	74655	100525	5.57%	1.042%
11	14.751	1943	1949	1957	rVB2	208882	310033	17.19%	3.215%
12	16.239	2197	2202	2214	rBV	599478	828932	45.95%	8.595%
13	16.968	2322	2326	2330	rBV2	16485	21652	1.20%	0.225%
14	17.486	2409	2414	2420	rBV	236588	342303	18.97%	3.549%
15	18.339	2555	2559	2567	rBV	128365	172978	9.59%	1.794%
16	19.598	2767	2773	2778	rBV2	67122	96439	5.35%	1.000%
17	20.068	2848	2853	2858	rBV	1575479	1803978	100.00%	18.706%
18	21.292	3058	3061	3066	rBV3	47915	56717	3.14%	0.588%
19	21.621	3113	3117	3126	rVB	339157	440140	24.40%	4.564%
20	23.950	3508	3513	3521	rVB	241432	445384	24.69%	4.618%

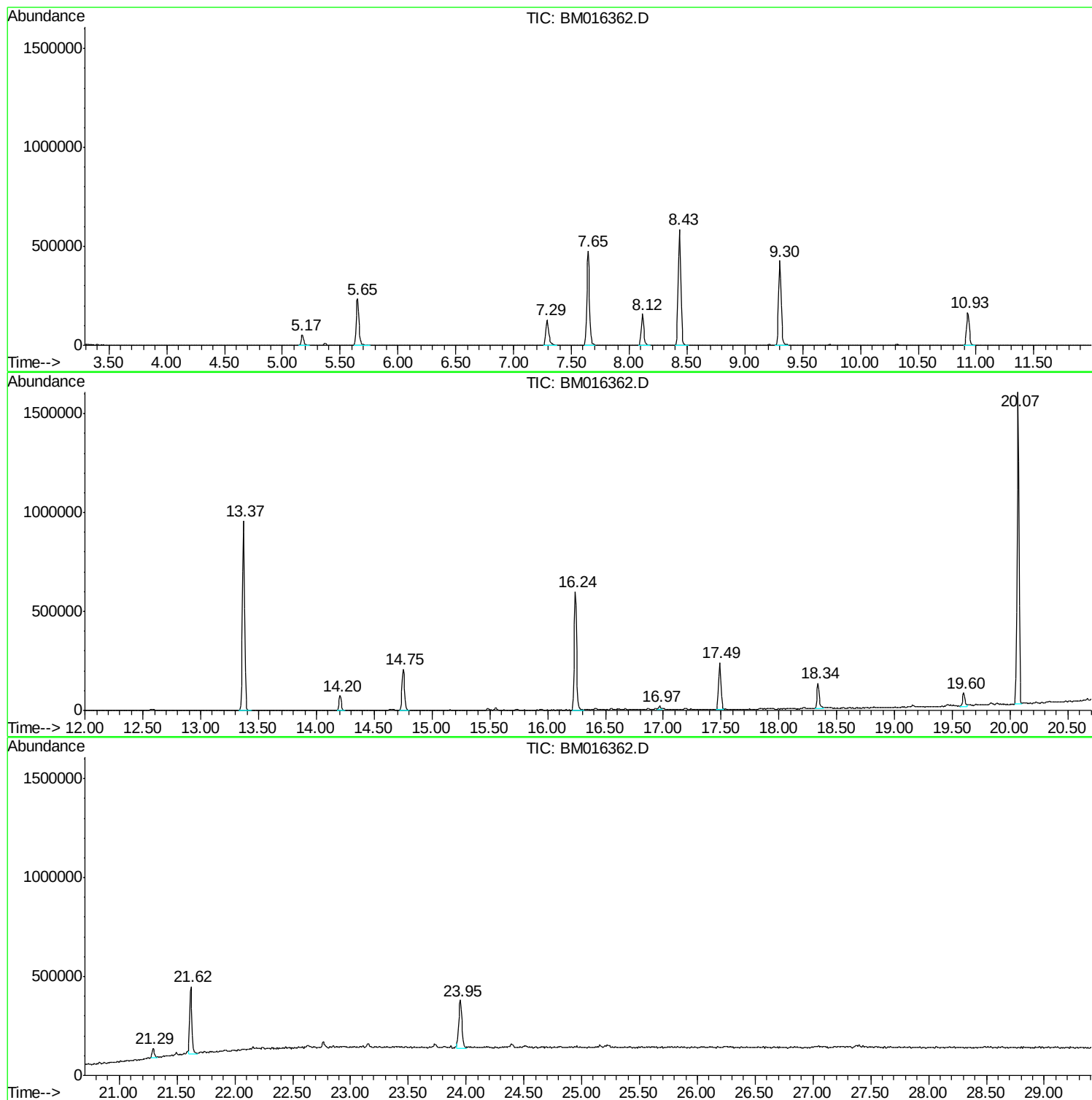
Sum of corrected areas: 9643996

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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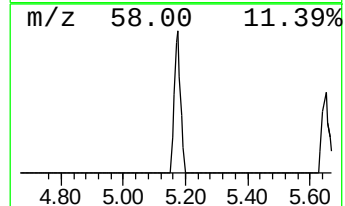
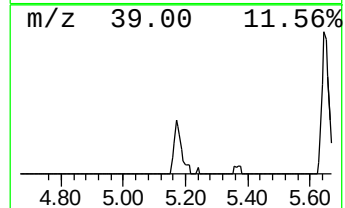
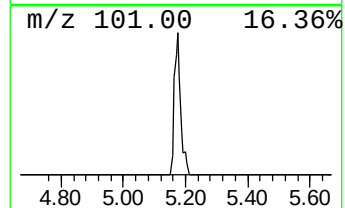
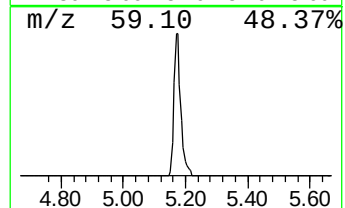
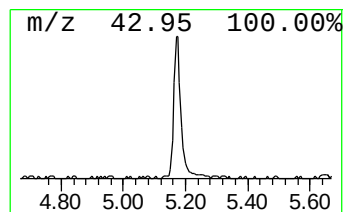
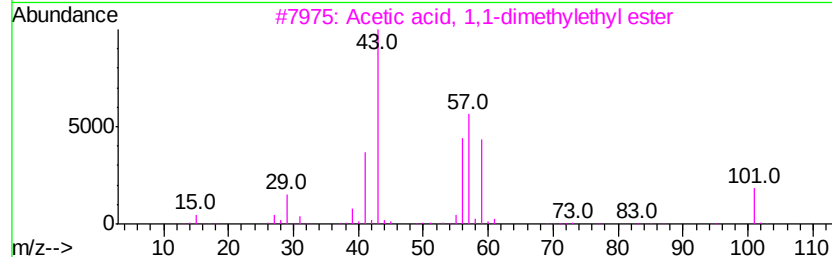
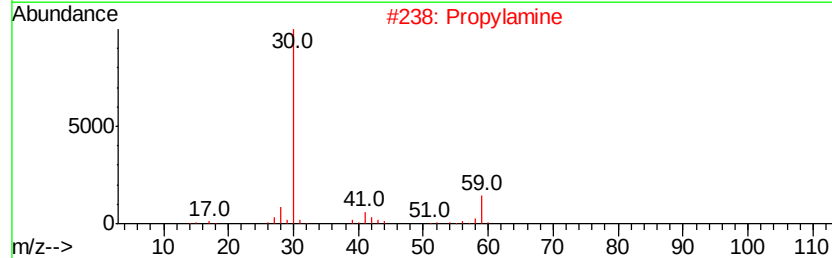
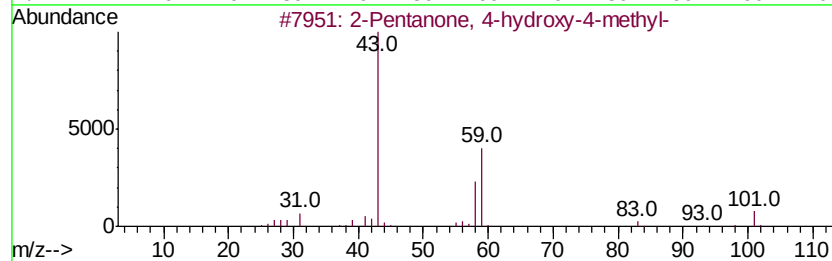
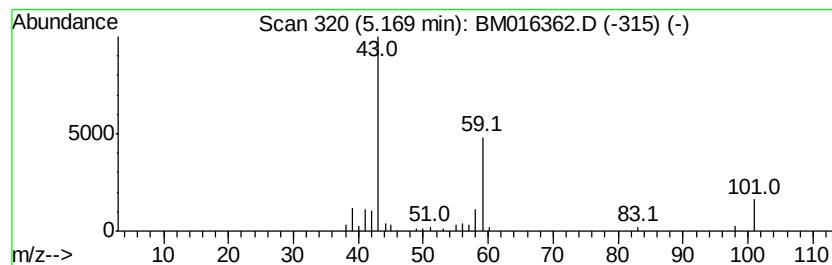
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	6.21 ng	78978	1,4-Dichlorobenzene-d4	8.12

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Propylamine	59	C3H9N	000107-10-8	40
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
4			2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	36
5			Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	25



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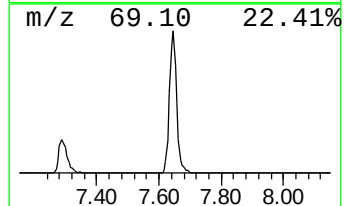
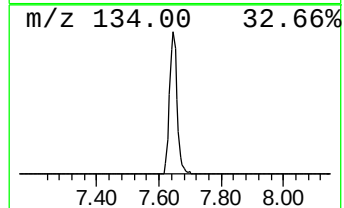
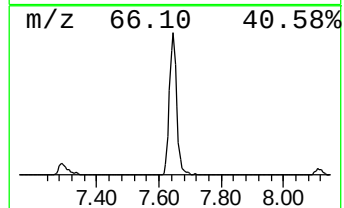
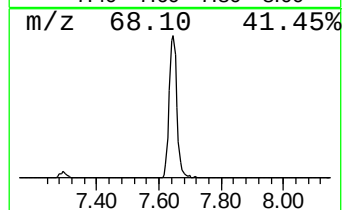
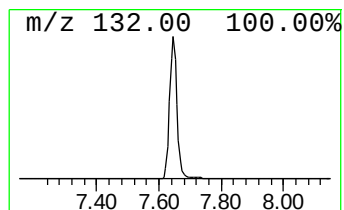
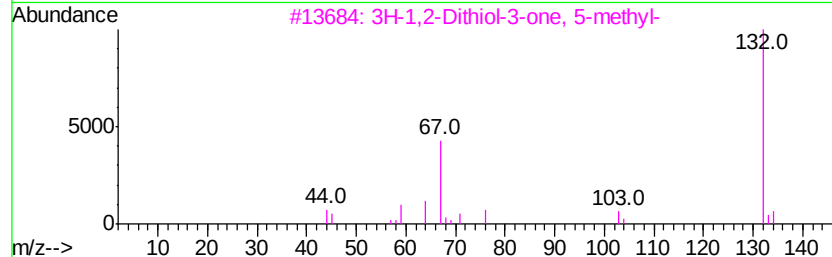
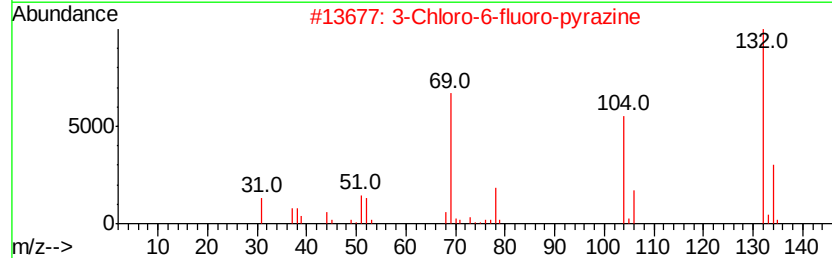
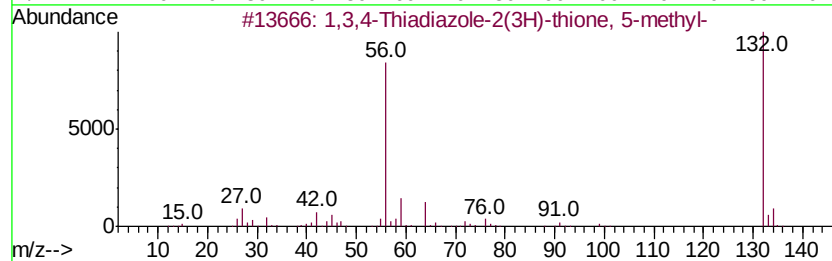
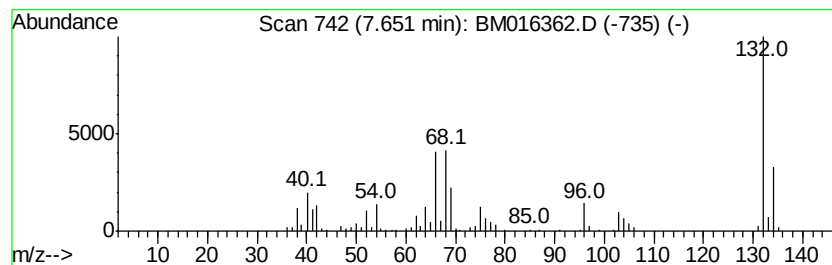
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Peak Number 2 unknown7.65 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	61.07 ng	777046	1,4-Dichlorobenzene-d4	8.12

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
2			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
3			3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
4			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
5			1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14



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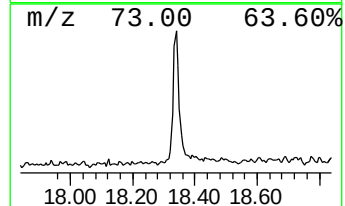
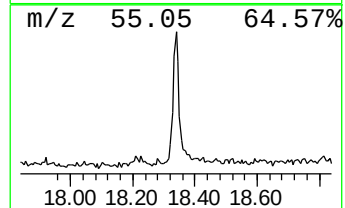
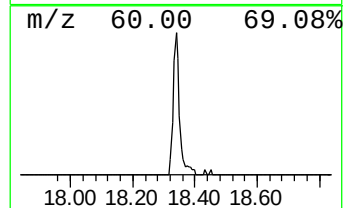
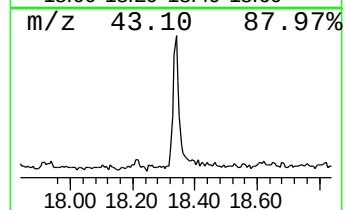
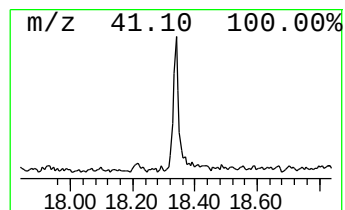
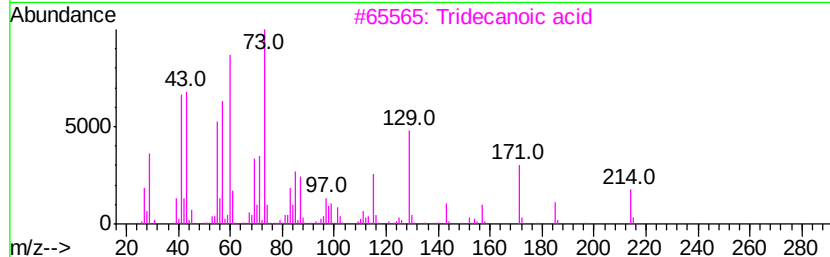
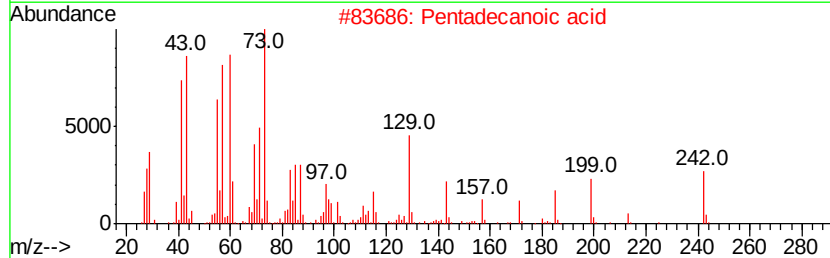
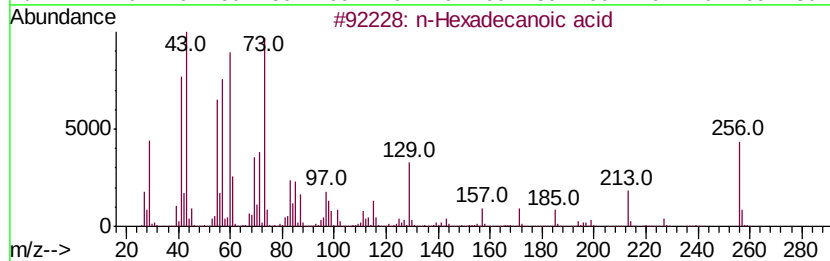
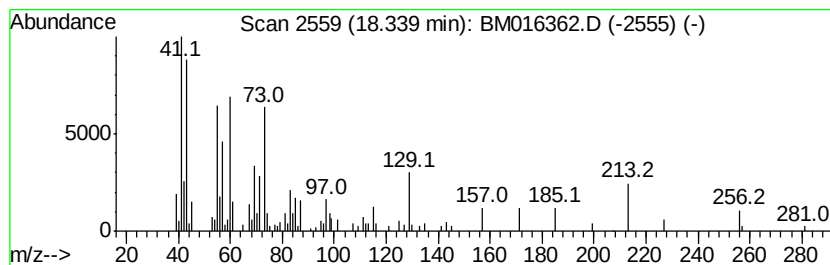
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.34	10.11 ng	172978	Phenanthrene-d10	17.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3		Tridecanoic acid	214	C13H26O2	000638-53-9	58
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5		Dodecanoic acid	200	C12H24O2	000143-07-7	43



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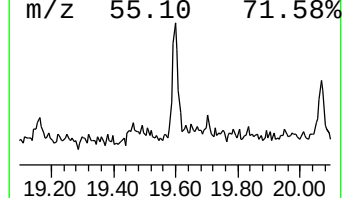
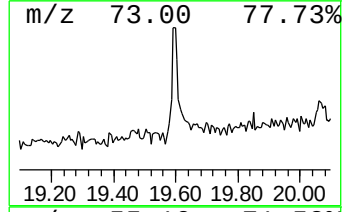
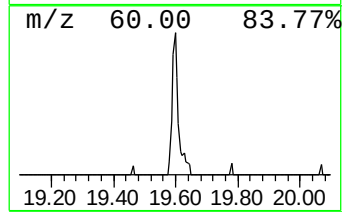
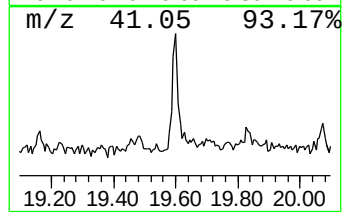
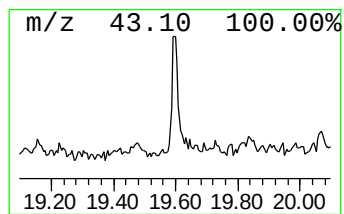
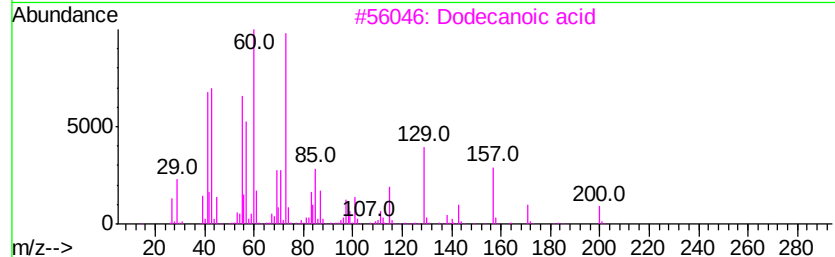
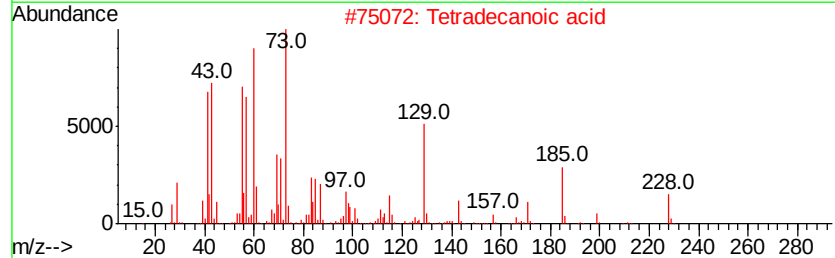
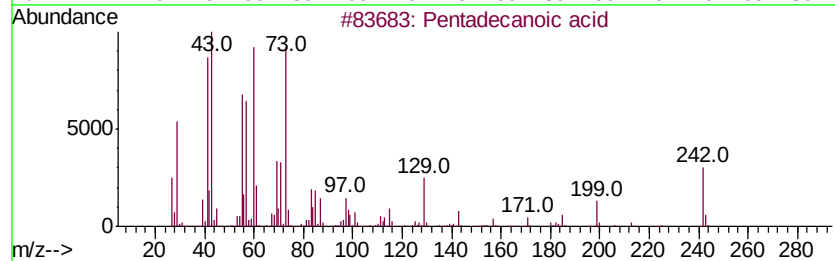
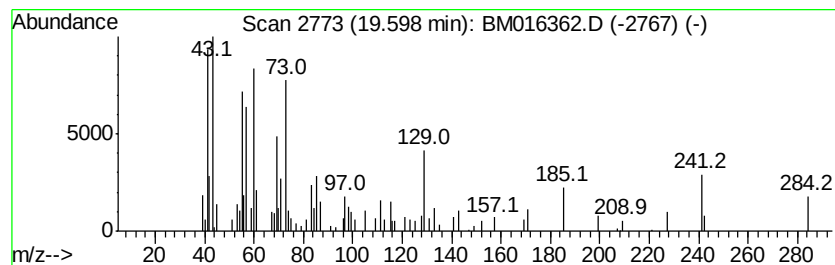
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Peak Number 5 Pentadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.60	4.38 ng	96439	Chrysene-d12	21.62

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	81
3		Dodecanoic acid	200	C12H24O2	000143-07-7	58
4		Tridecanoic acid	214	C13H26O2	000638-53-9	52
5		n-Decanoic acid	172	C10H20O2	000334-48-5	47



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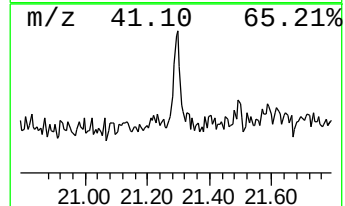
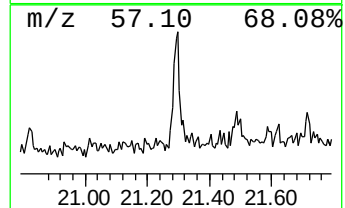
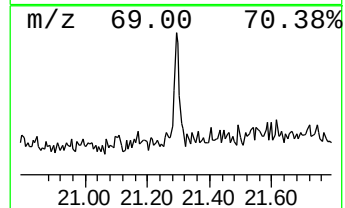
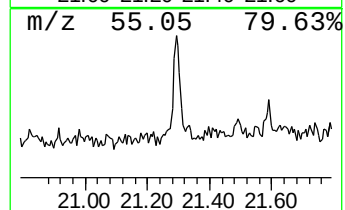
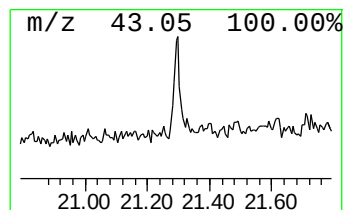
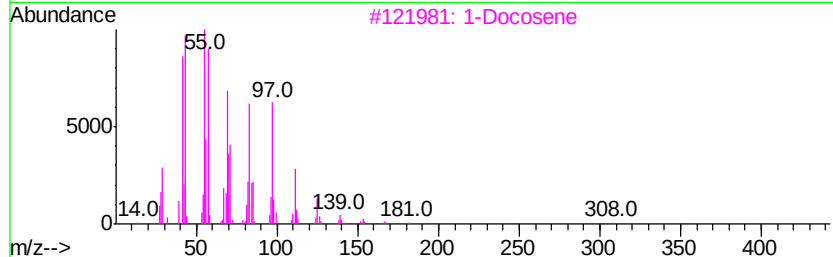
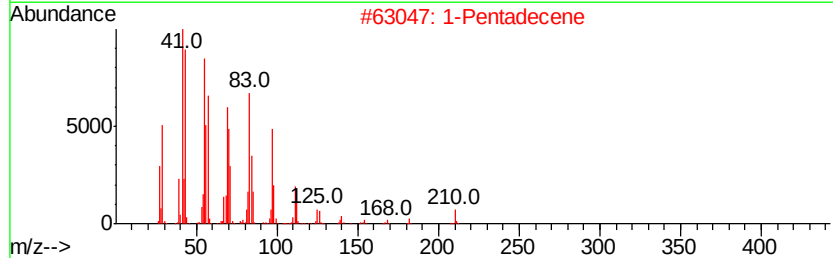
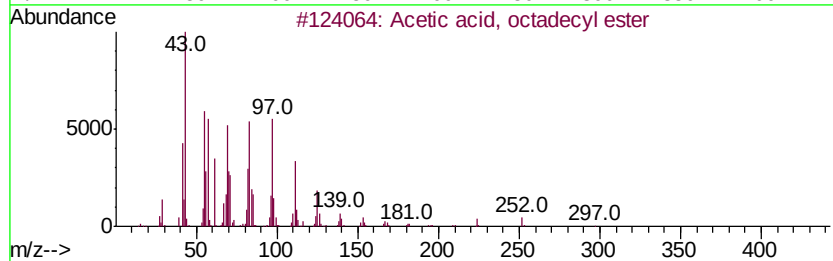
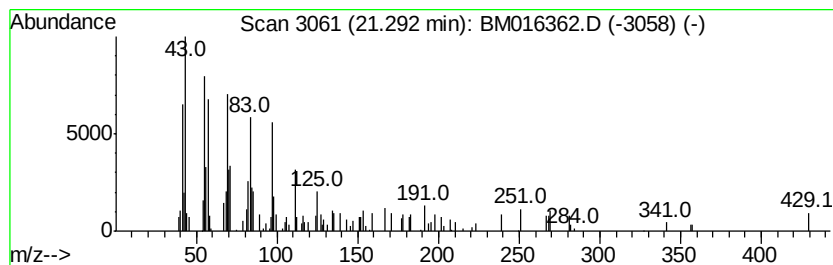
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Peak Number 6 Acetic acid, octadecyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.29	2.58 ng	56717	Chrysene-d12	21.62	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	87
2	1-Pentadecene	210	C15H30	013360-61-7	86
3	1-Docosene	308	C22H44	001599-67-3	83
4	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	76
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	76



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TIC Library : C:\DATABASE\NIST02.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.17	6.2	ng	78978	1	8.12	254493	20.0
unknown7.65	7.65	61.1	ng	777046	1	8.12	254493	20.0
n-Hexadecanoic acid	18.34	10.1	ng	172978	4	17.49	342303	20.0
Pentadecanoic acid	19.60	4.4	ng	96439	5	21.62	440140	20.0
Acetic acid, octa...	21.29	2.6	ng	56717	5	21.62	440140	20.0