

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121818\
 Data File : BM018280.D
 Acq On : 18 Dec 2018 20:36
 Operator : JU/SJ
 Sample : J6377-19
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 P001-SD007-0006-01

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-BM121518.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	3.363	77	81	89	rBV	41345	58685	1.33%	0.165%
2	4.681	300	305	311	rBV	87831	119027	2.69%	0.334%
3	5.122	374	380	392	rBV	2693947	3711716	83.94%	10.423%
4	6.693	640	647	661	rBV	2507713	4100011	92.72%	11.513%
5	7.028	697	704	714	rBV	2718785	4108484	92.91%	11.537%
6	7.487	771	782	791	rBV	506721	789347	17.85%	2.217%
7	7.798	828	835	848	rBV	1930919	2943650	66.57%	8.266%
8	8.645	972	979	1003	rBV	1418302	2374950	53.71%	6.669%
9	10.251	1245	1252	1271	rBV	551114	1009799	22.84%	2.836%
10	12.751	1670	1677	1693	rBV	3037636	4422052	100.00%	12.417%
11	13.622	1818	1825	1836	rBV	135153	228962	5.18%	0.643%
12	14.145	1908	1914	1931	rVB2	739774	1133528	25.63%	3.183%
13	15.651	2164	2170	2186	rBV	1914319	2796717	63.24%	7.853%
14	16.910	2378	2384	2397	rBV	705530	1066669	24.12%	2.995%
15	17.821	2534	2539	2547	rBV	133855	205482	4.65%	0.577%
16	19.115	2755	2759	2765	rBV3	56061	84967	1.92%	0.239%
17	19.562	2830	2835	2845	rBV	2883444	3591455	81.22%	10.085%
18	20.856	3051	3055	3061	rBV	176571	257427	5.82%	0.723%
19	21.133	3097	3102	3113	rBV	852535	1191083	26.94%	3.345%
20	21.745	3203	3206	3212	rVB5	113877	169879	3.84%	0.477%
21	22.156	3274	3276	3279	rBV4	48543	51273	1.16%	0.144%
22	23.292	3463	3469	3479	rBV	664710	1197012	27.07%	3.361%

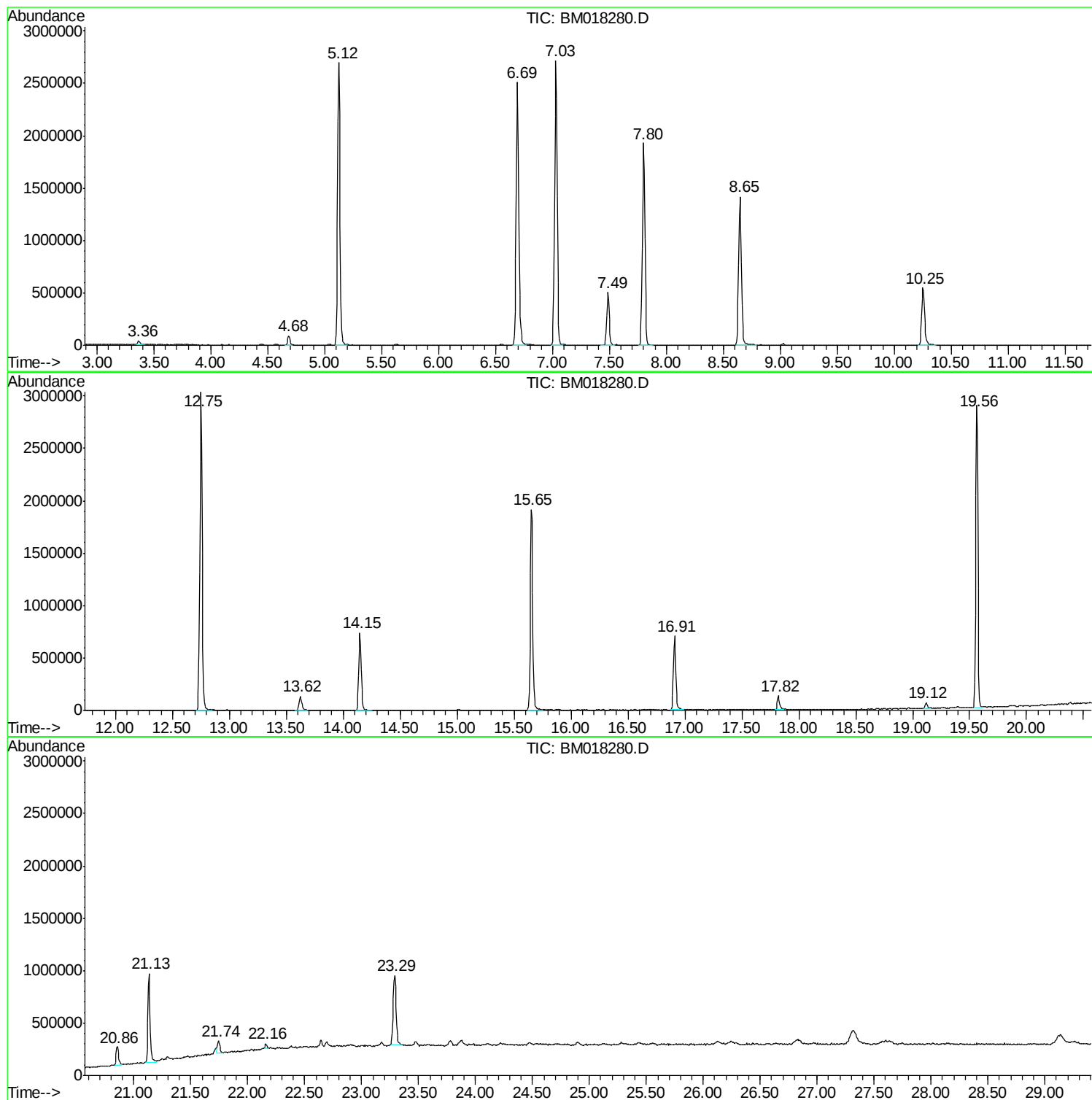
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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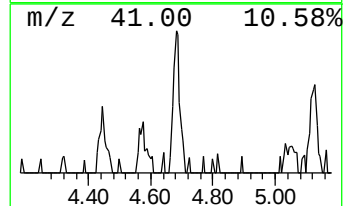
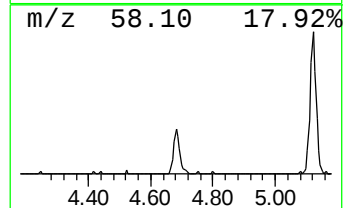
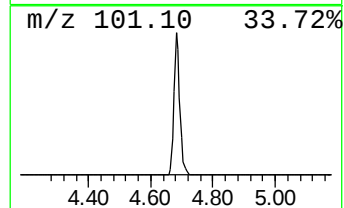
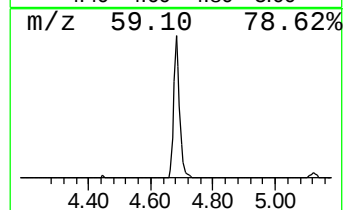
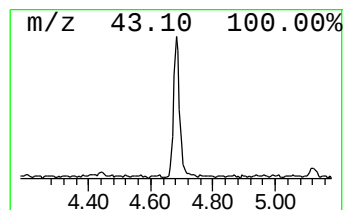
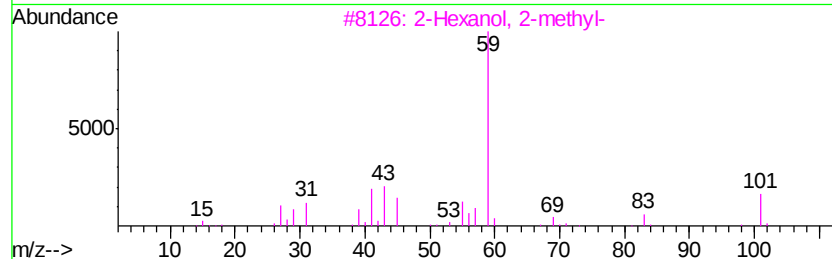
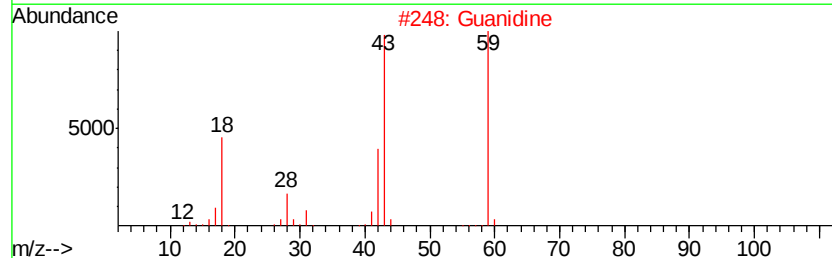
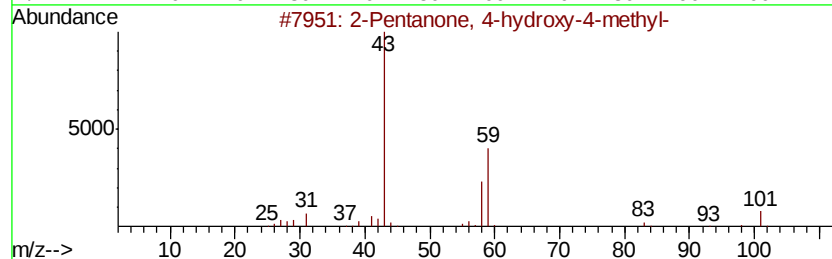
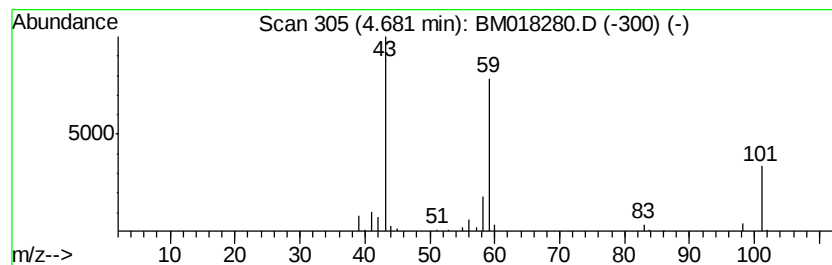
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.68	3.02 ng	119027	1,4-Dichlorobenzene-d4	7.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Guanidine	59	CH5N3	000113-00-8	50
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	42
4			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	37
5			1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	28



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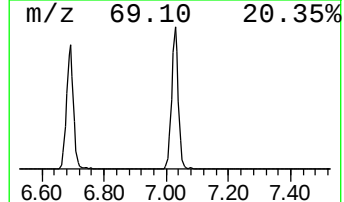
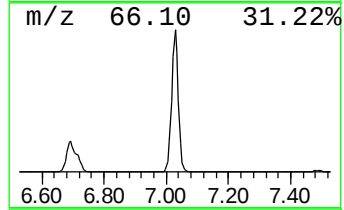
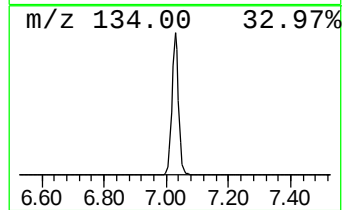
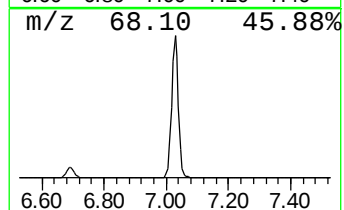
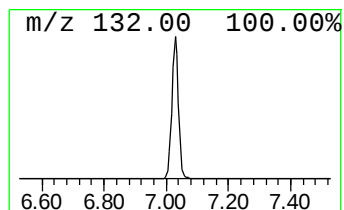
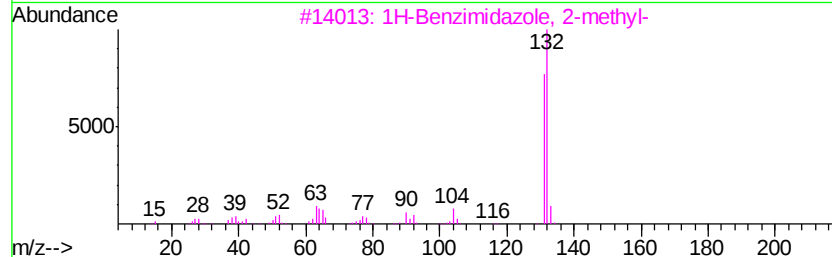
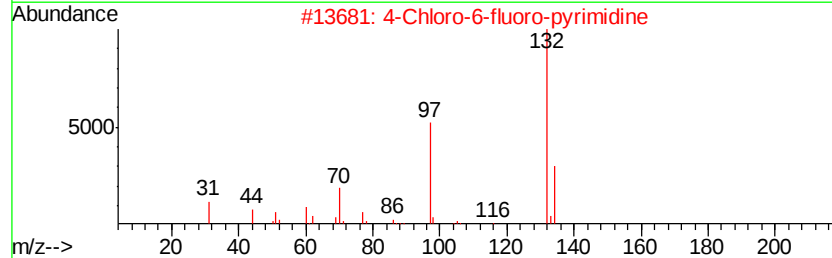
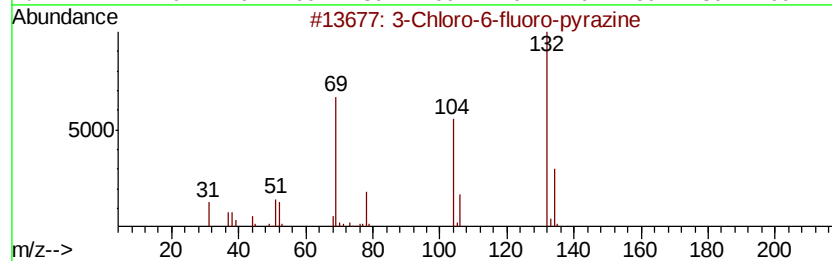
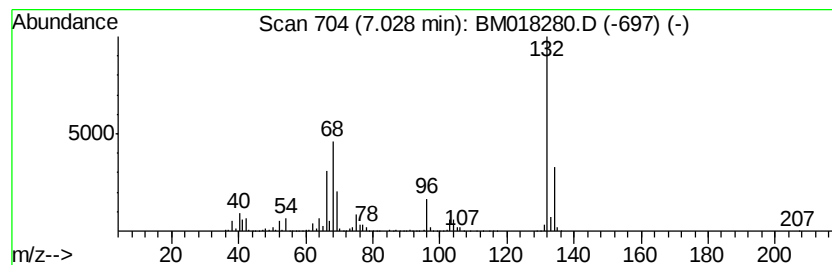
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Peak Number 2 unknown7.03 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.03	104.10 ng	4108480	1,4-Dichlorobenzene-d4	7.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	10



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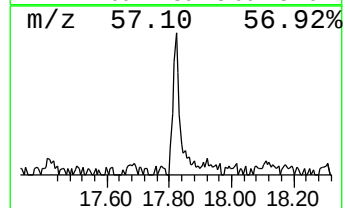
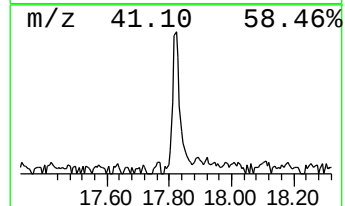
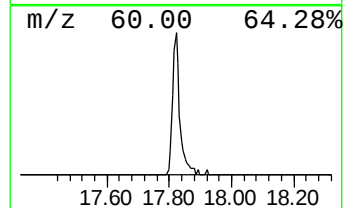
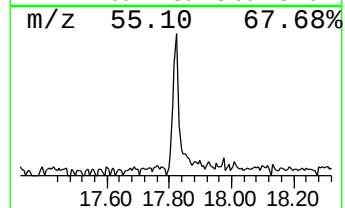
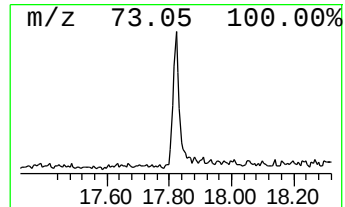
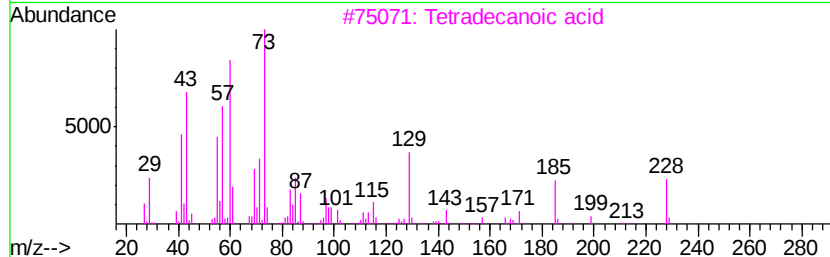
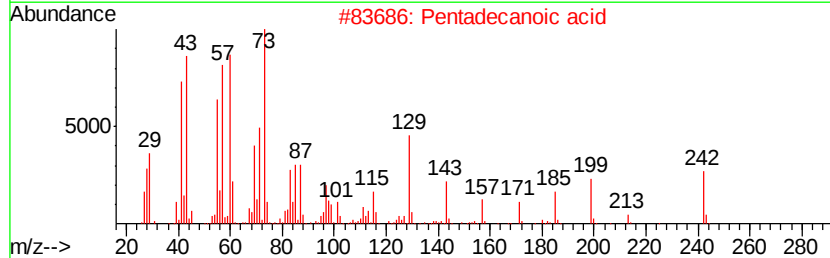
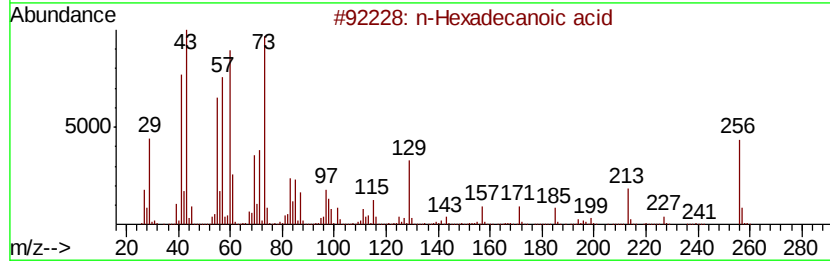
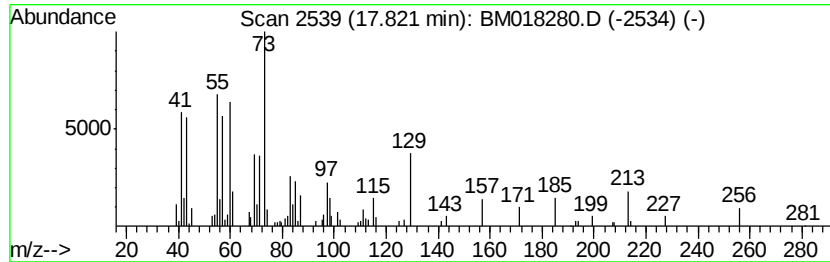
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.82	3.85 ng	205482	Phenanthrene-d10	16.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	59
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	50
4		Dodecanoic acid	200	C12H24O2	000143-07-7	47
5		Tridecanoic acid	214	C13H26O2	000638-53-9	47



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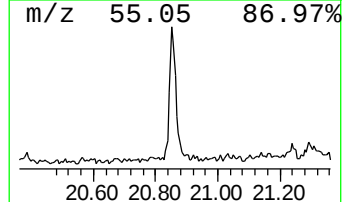
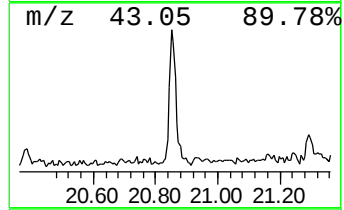
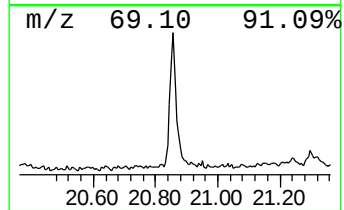
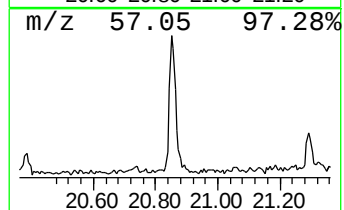
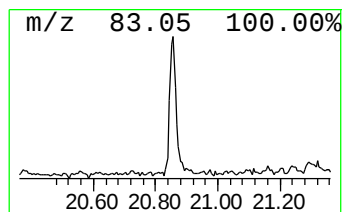
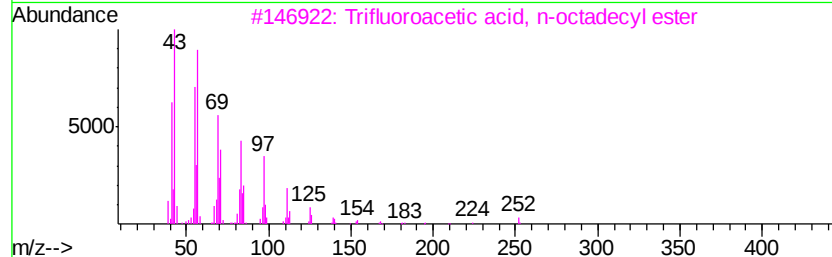
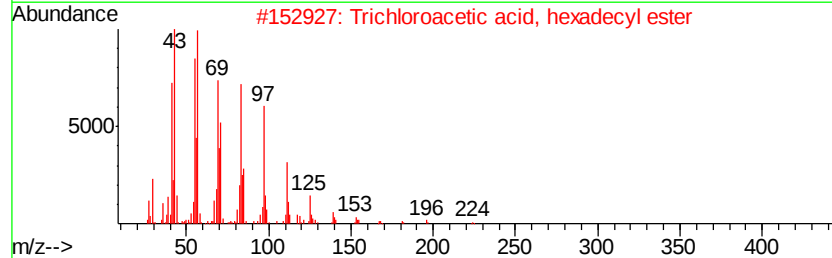
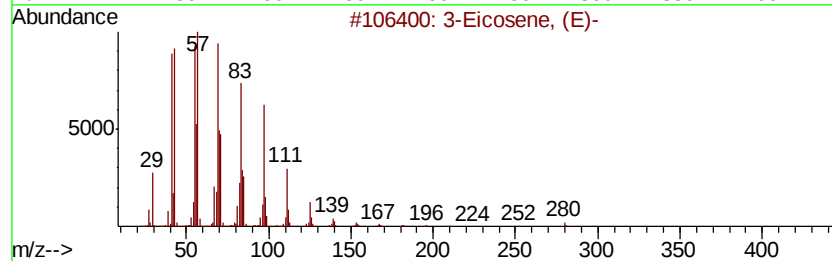
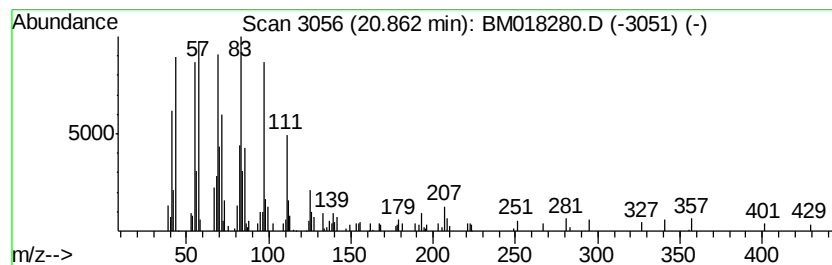
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Peak Number 5 3-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.86	4.32 ng	257427	Chrysene-d12	21.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Eicosene, (E)-	280	C20H40	074685-33-9	92
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3		Trifluoroacetic acid, n-octadecyl...	366	C20H37F3O2	079392-43-1	74
4		Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	74
5		1-Docosene	308	C22H44	001599-67-3	64



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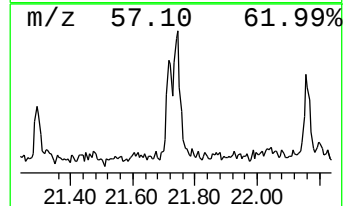
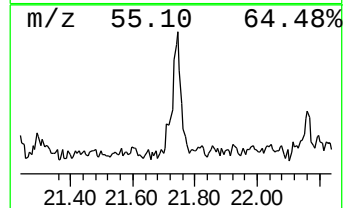
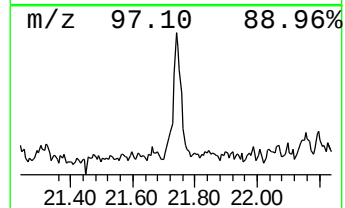
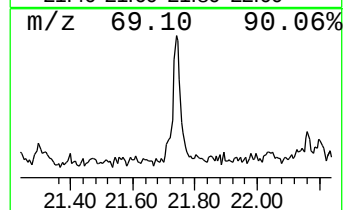
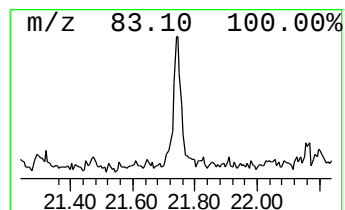
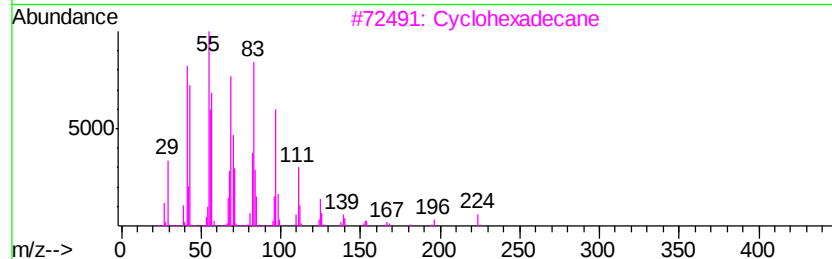
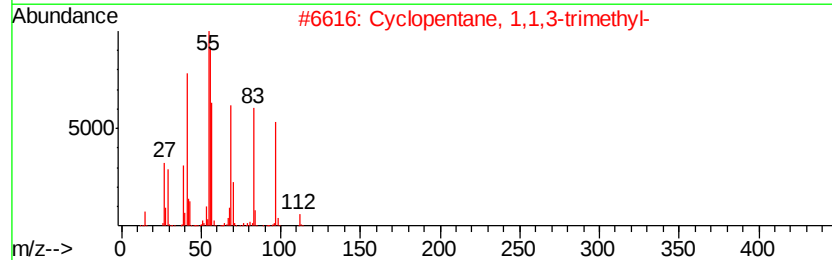
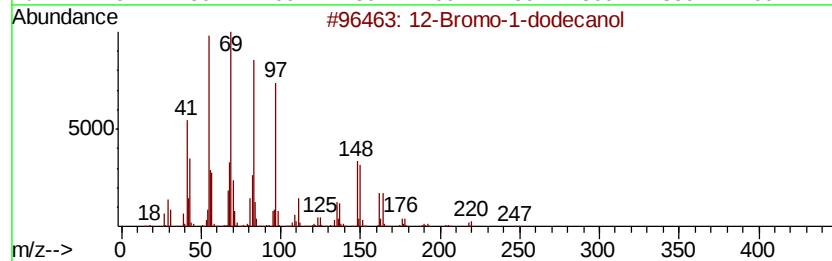
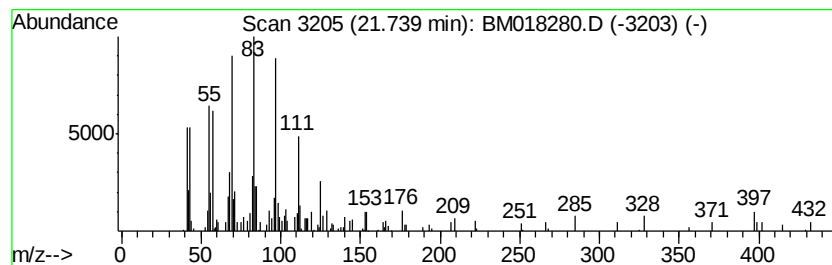
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Peak Number 6 12-Bromo-1-dodecanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.74	2.85 ng	169879	Chrysene-d12	21.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		12-Bromo-1-dodecanol	264	C12H25BrO	003344-77-2	59
2		Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	58
3		Cyclohexadecane	224	C16H32	000295-65-8	43
4		3-Hexene, 3-ethyl-2,5-dimethyl-	140	C10H20	062338-08-3	43
5		3-Heptene, 4-propyl-	140	C10H20	004485-13-6	43



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.68	3.0	ng	119027	1	7.49	789347	20.0
unknown7.03	7.03	104.1	ng	4108480	1	7.49	789347	20.0
n-Hexadecanoic acid	17.82	3.9	ng	205482	4	16.91	1066670	20.0
3-Eicosene, (E)-	20.86	4.3	ng	257427	5	21.13	1191080	20.0
12-Bromo-1-dodecanol	21.74	2.9	ng	169879	5	21.13	1191080	20.0