

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112215\
 Data File : BF083192.D
 Acq On : 23 Nov 2015 7:27
 Operator : UM/IZ
 Sample : G4437-05
 Misc :
 ALS Vial : 78 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-25

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:\HPCHEM1\BNA_F\METHODS\8270-BF112115.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	4.787	242	245	261	rVB	1018393	1440548	20.53%	2.919%
2	5.256	283	286	297	rBV	2214109	3458980	49.28%	7.009%
3	6.307	376	378	385	rBV	1990459	2239083	31.90%	4.537%
4	6.421	385	388	391	rBV	5392020	5472188	77.97%	11.088%
5	6.650	405	408	410	rBV	1335519	1300057	18.52%	2.634%
6	6.810	419	422	424	rBV	5156869	5414261	77.14%	10.970%
7	7.176	451	454	455	rBV	87034	94956	1.35%	0.192%
8	7.222	455	458	461	rVV	4185924	4546691	64.78%	9.213%
9	7.267	461	462	464	rVV	95419	89996	1.28%	0.182%
10	7.519	482	484	486	rVB2	83229	90146	1.28%	0.183%
11	7.930	518	520	523	rBV	1139677	1592928	22.70%	3.228%
12	8.467	565	567	570	rBV	170042	178123	2.54%	0.361%
13	9.016	612	615	618	rBV	6046229	7018356	100.00%	14.221%
14	9.416	647	650	654	rVB	51331	74543	1.06%	0.151%
15	9.679	671	673	676	rBV	1328012	1591786	22.68%	3.225%
16	9.930	692	695	699	rVB3	45769	72135	1.03%	0.146%
17	10.468	740	742	745	rBV2	2841627	3857501	54.96%	7.816%
18	11.153	800	802	805	rBV	1132753	1451527	20.68%	2.941%
19	11.713	848	851	856	rBV2	206056	269371	3.84%	0.546%
20	12.411	909	912	917	rBV3	27103	77050	1.10%	0.156%
21	12.491	917	919	922	rBV	348271	385105	5.49%	0.780%
22	12.754	939	942	944	rBV	4368391	6085218	86.70%	12.330%
23	13.325	990	992	994	rBV2	90718	94496	1.35%	0.191%
24	13.782	1030	1032	1035	rBV	1518599	1401841	19.97%	2.840%
25	15.154	1149	1152	1155	rBV	736991	1056180	15.05%	2.140%

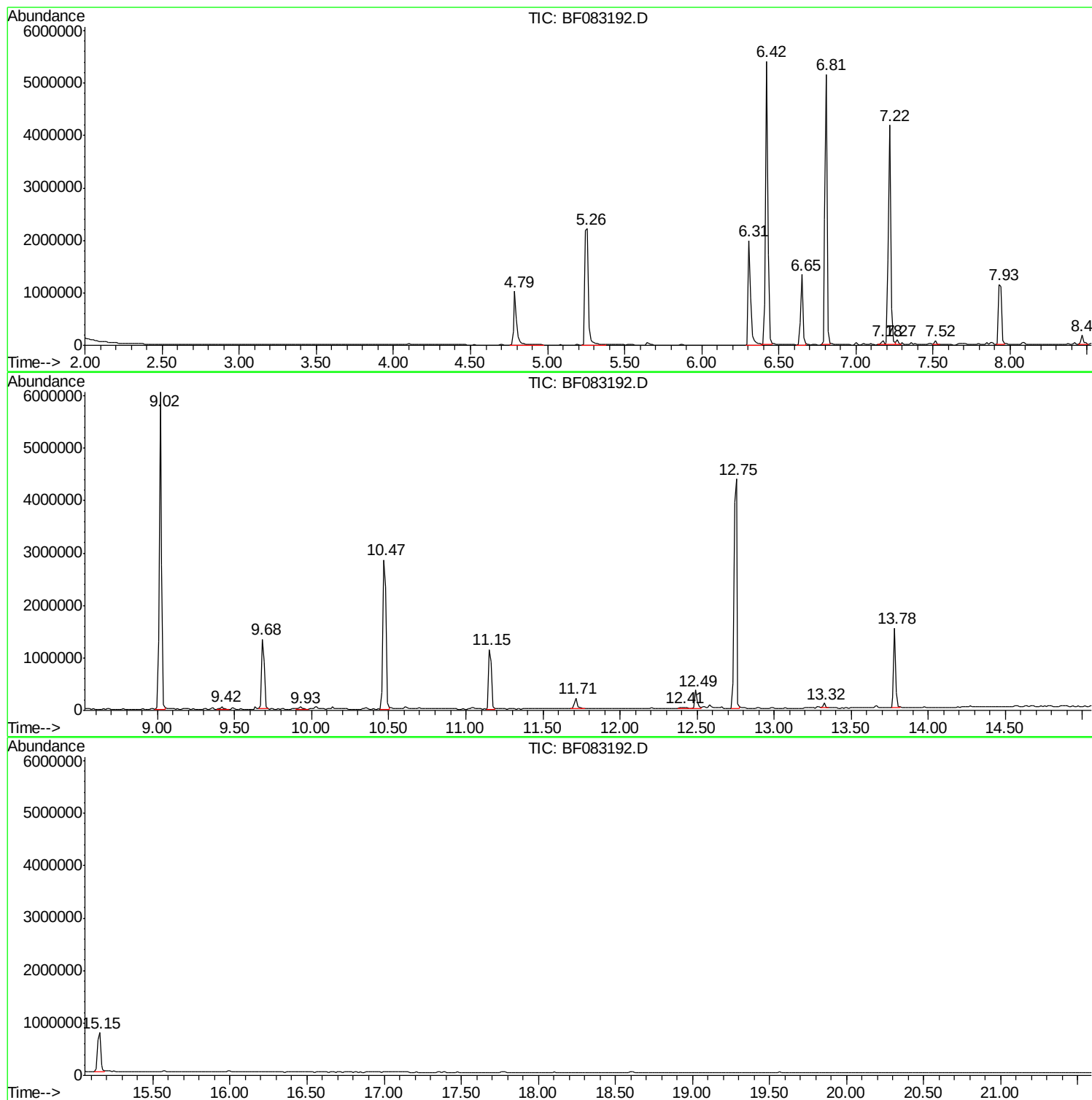
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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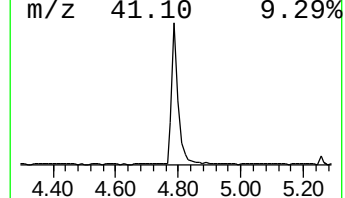
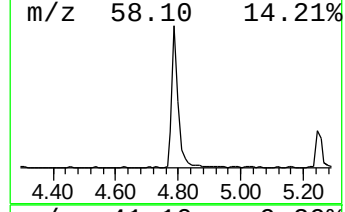
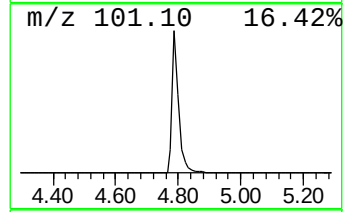
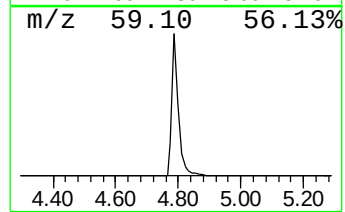
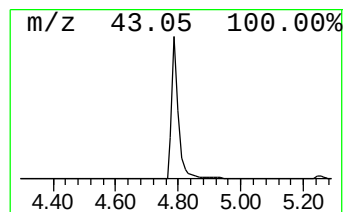
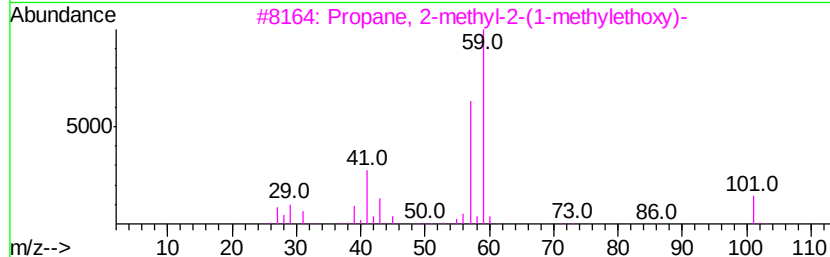
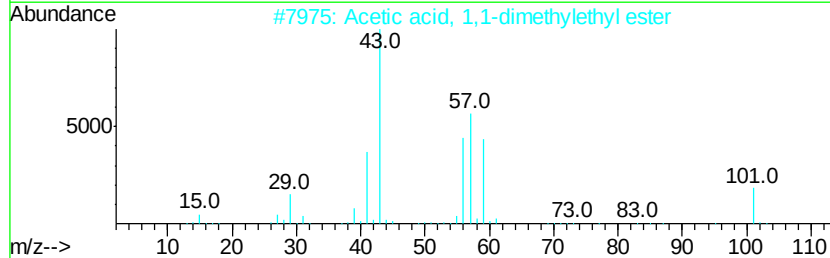
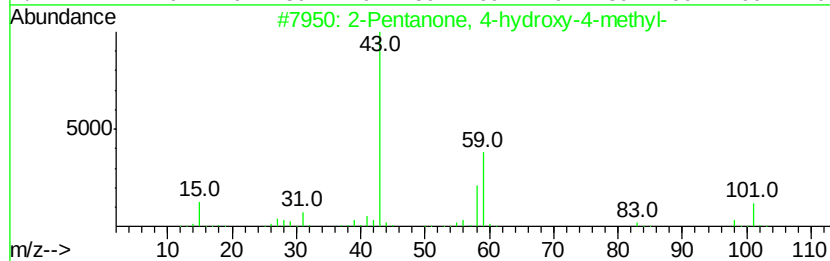
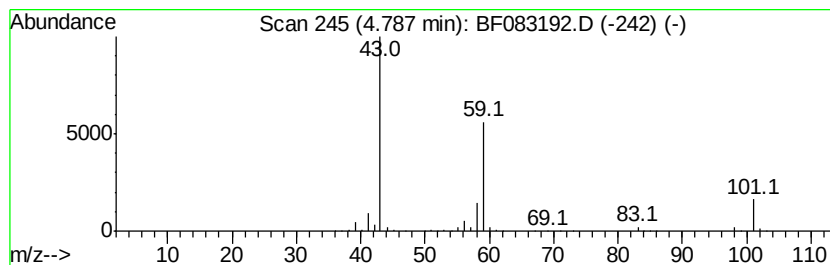
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.79	22.16 ng	1440550	1,4-Dichlorobenzene-d4	6.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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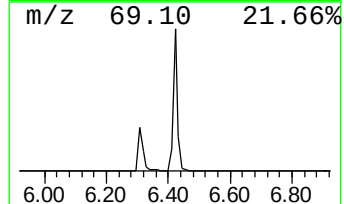
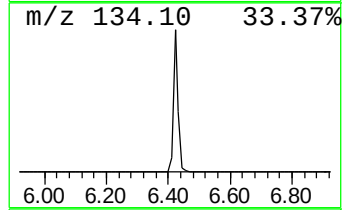
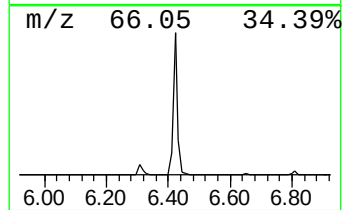
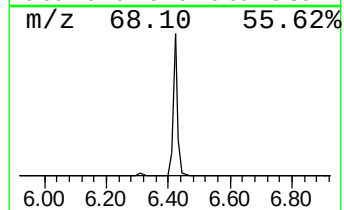
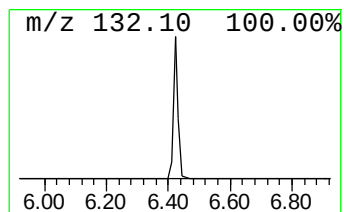
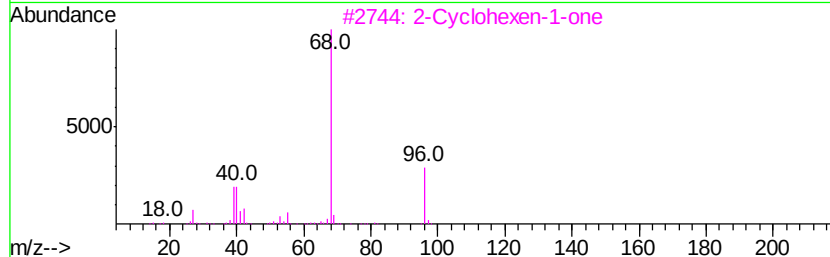
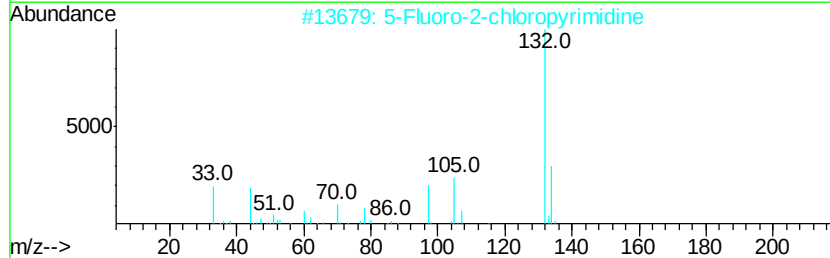
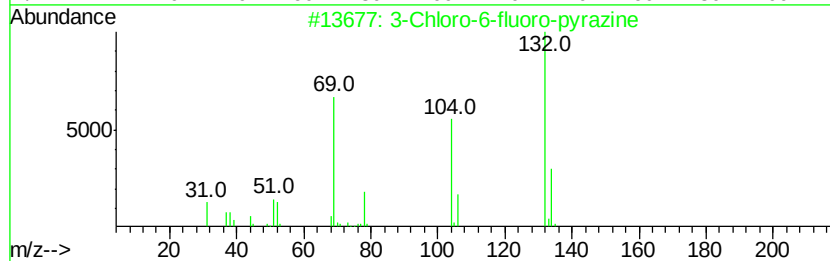
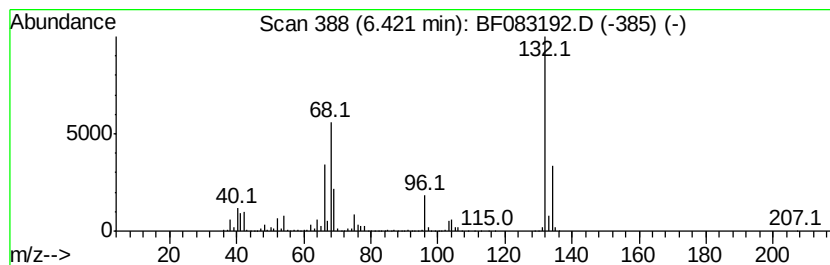
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	84.18 ng	5472190	1,4-Dichlorobenzene-d4	6.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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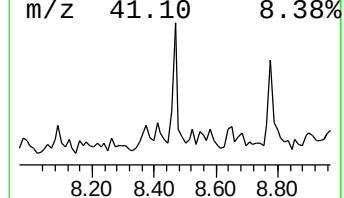
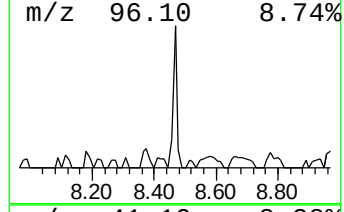
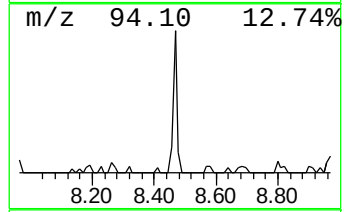
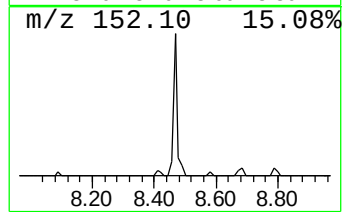
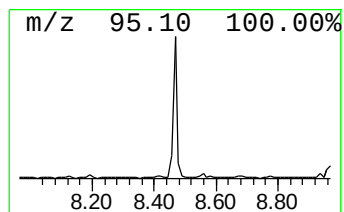
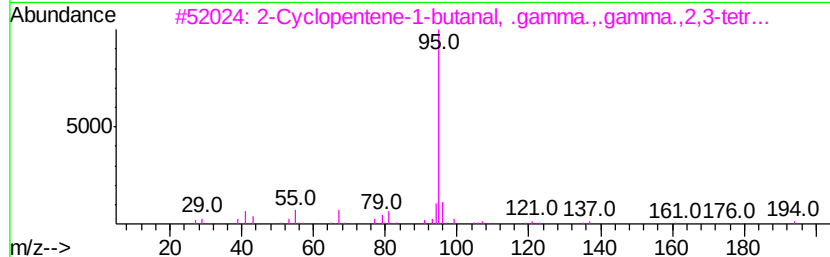
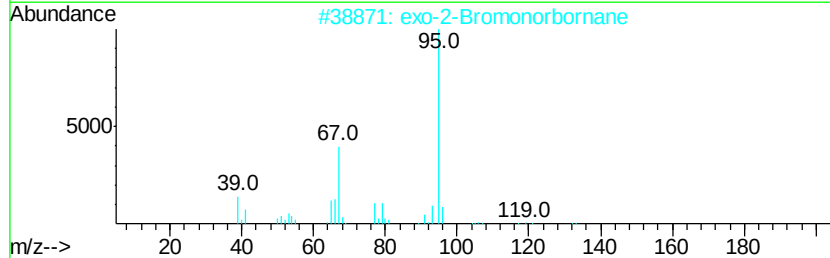
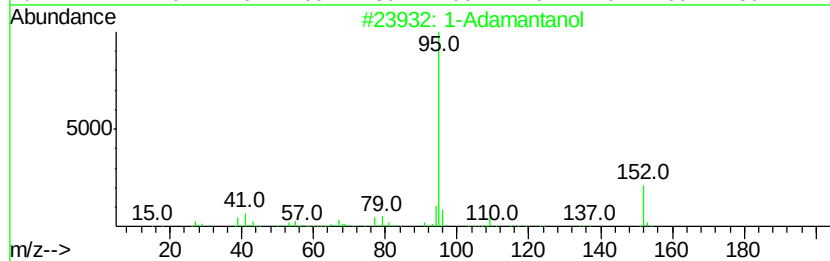
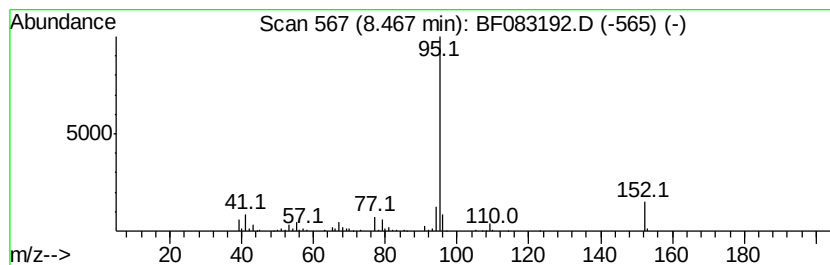
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Peak Number 4 1-Adamantanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.47	2.24 ng	178123	Naphthalene-d8	7.94

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Adamantanol		152	C10H16O	000768-95-6	91
2	exo-2-Bromonorbornane		174	C7H11Br	002534-77-2	45
3	2-Cyclopentene-1-butanal, .gamma...		194	C13H22O	060714-25-2	39
4	1-(3H-Imidazol-4-yl)-ethanone		110	C5H6N2O	061985-25-9	33
5	1H-Pyrrole-2-carboxaldehyde		95	C5H5NO	001003-29-8	9



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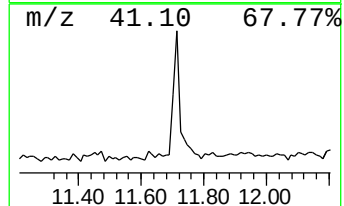
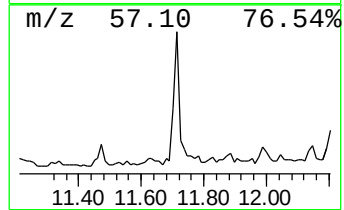
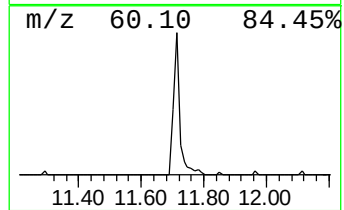
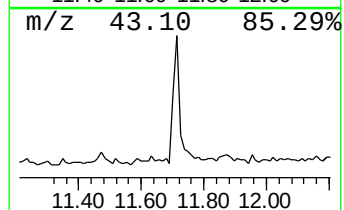
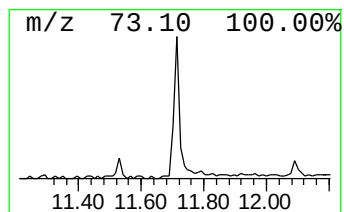
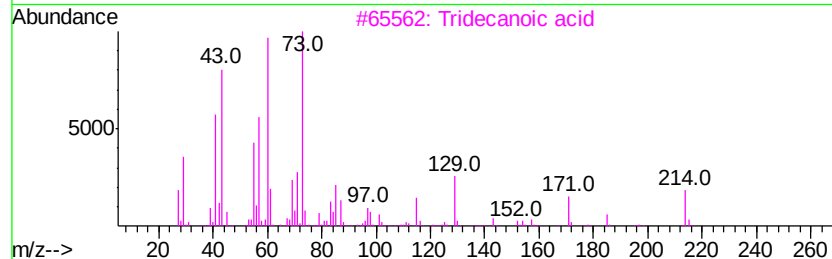
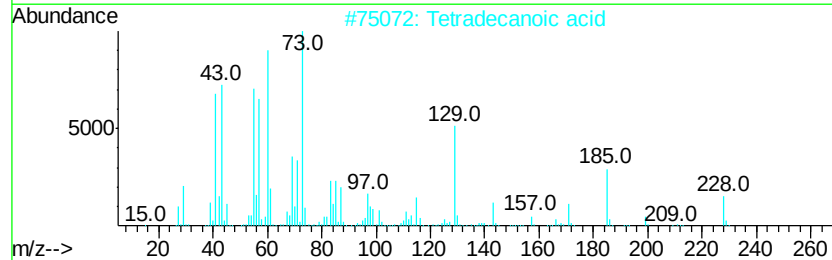
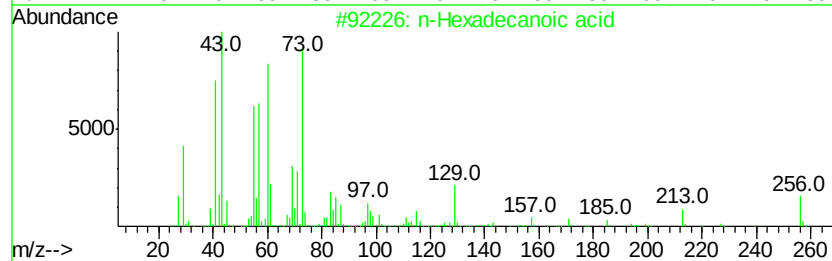
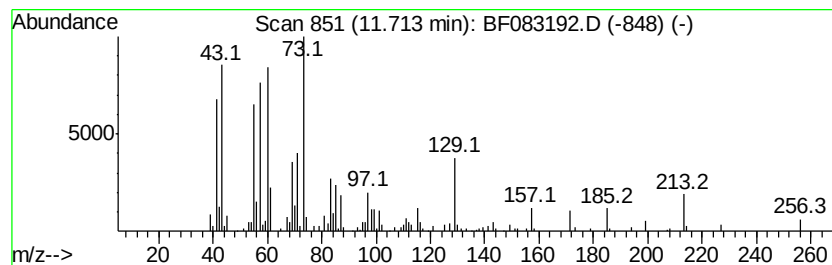
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.71	3.71 ng	269371	Phenanthrene-d10	11.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3		Tridecanoic acid	214	C13H26O2	000638-53-9	81
4		Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	42
5		Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	11



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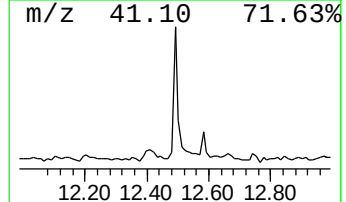
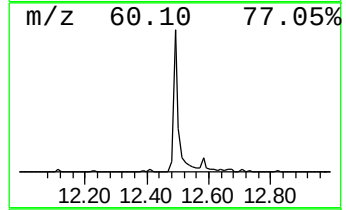
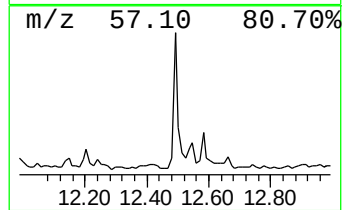
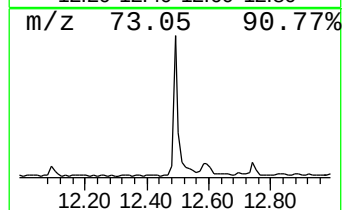
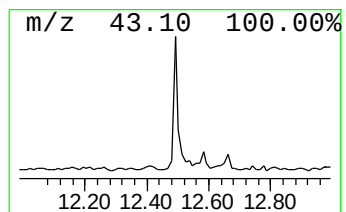
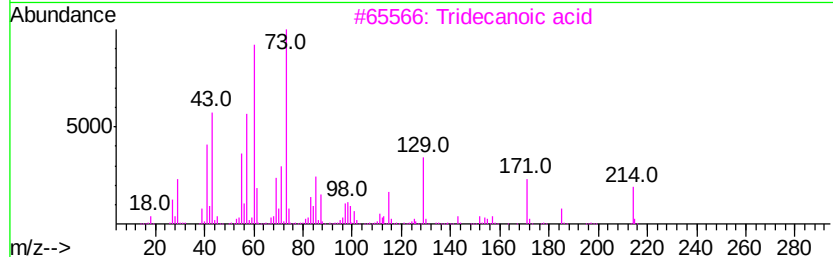
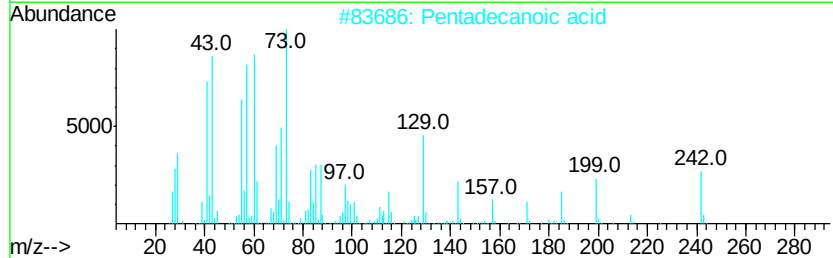
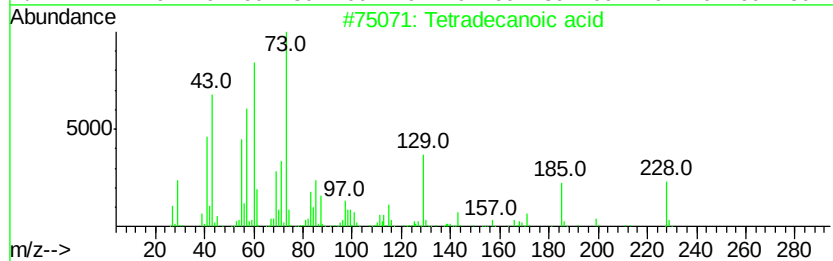
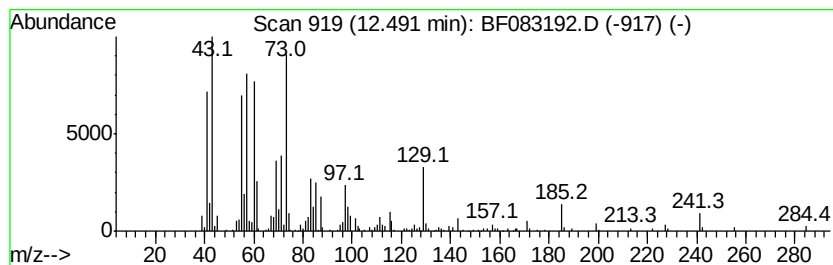
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Peak Number 6 Tetradecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.49	5.49 ng	385105	Chrysene-d12	13.78	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Amvl Nitrite	117	C5H11NO2	000110-46-3	35
5	Hexadecane	226	C16H34	000544-76-3	11



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.79	22.2	ng	1440550	1	6.65	1300060	20.0
unknown6.42	6.42	84.2	ng	5472190	1	6.65	1300060	20.0
1-Adamantanol	8.47	2.2	ng	178123	2	7.94	1592930	20.0
n-Hexadecanoic acid	11.71	3.7	ng	269371	4	11.15	1451530	20.0
Tetradecanoic acid	12.49	5.5	ng	385105	5	13.78	1401840	20.0