

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120516\
 Data File : BF091428.D
 Acq On : 5 Dec 2016 20:00
 Operator : UM/SJ
 Sample : H5838-07
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-115

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-BF112916.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	5.030	237	240	243	rBV	359910	536847	9.69%	1.449%
2	5.442	274	276	279	rBV	1934148	2005891	36.20%	5.413%
3	6.470	363	366	368	rBV	1426277	1226631	22.13%	3.310%
4	6.619	376	379	381	rBV	3507021	4080341	73.63%	11.011%
5	6.847	397	399	401	rBV	1041124	883626	15.95%	2.385%
6	7.007	410	413	415	rBV	3949965	3764792	67.94%	10.160%
7	7.407	445	448	451	rBV	2111013	3158708	57.00%	8.524%
8	8.128	509	511	514	rBV	855703	1063510	19.19%	2.870%
9	9.213	603	606	608	rBV	5310882	5171379	93.32%	13.956%
10	9.888	662	665	667	rBV	1570767	1416481	25.56%	3.823%
11	10.676	731	734	736	rBV	3735853	3972172	71.68%	10.719%
12	11.362	792	794	797	rVB	1141046	1343045	24.24%	3.624%
13	11.899	839	841	843	rBV	139241	132223	2.39%	0.357%
14	12.688	907	910	916	rBV	180787	210515	3.80%	0.568%
15	12.779	916	918	922	rVV	310013	266056	4.80%	0.718%
16	12.962	931	934	936	rBV	4542091	5541690	100.00%	14.955%
17	13.511	980	982	989	rVB	238942	237526	4.29%	0.641%
18	13.854	1009	1012	1017	rBV	47620	61054	1.10%	0.165%
19	14.002	1022	1025	1027	rBV	1043516	1157654	20.89%	3.124%
20	15.420	1146	1149	1152	rBV	596053	825904	14.90%	2.229%

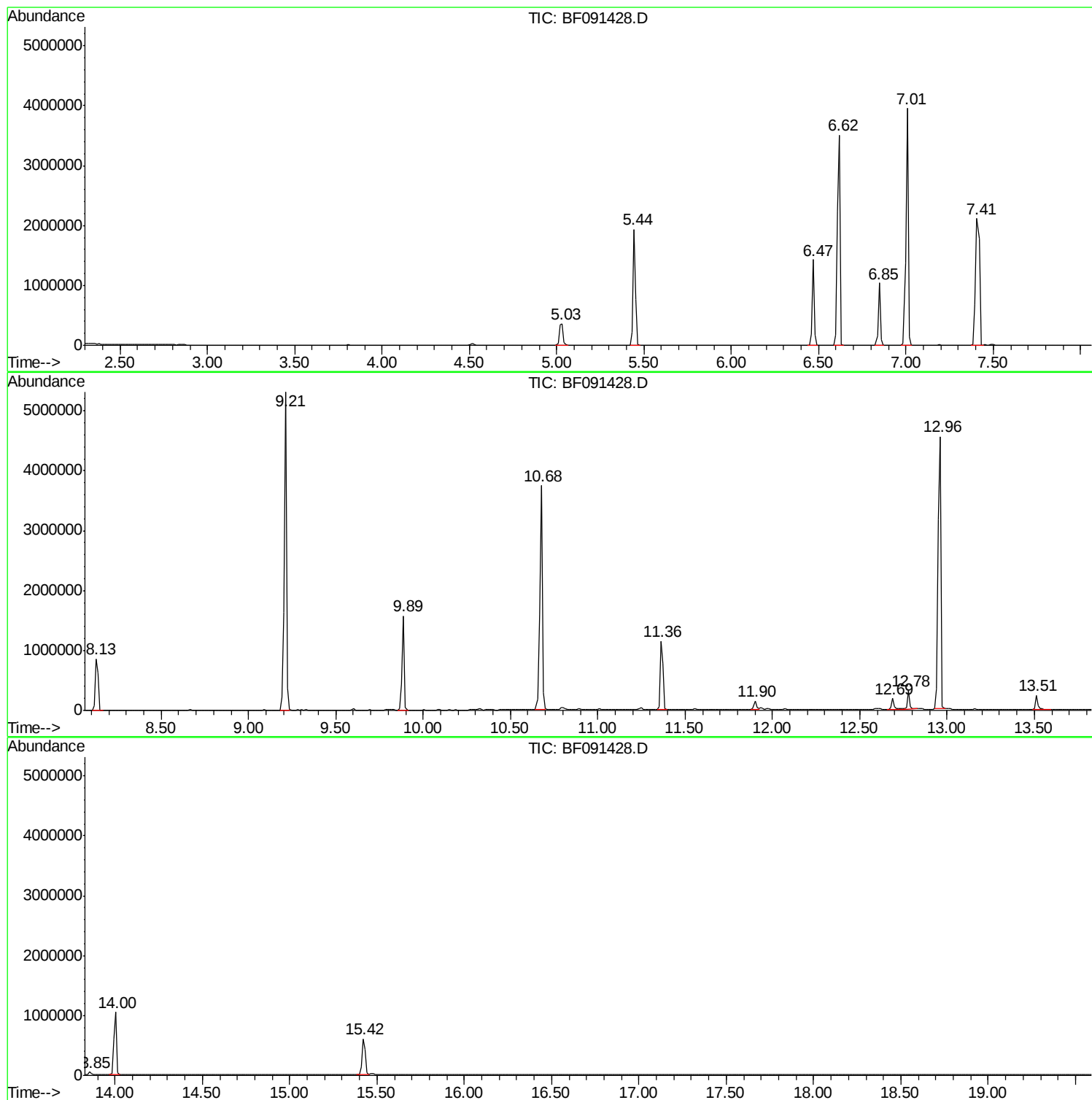
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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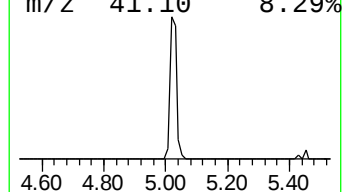
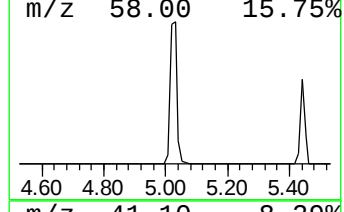
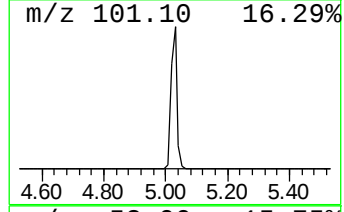
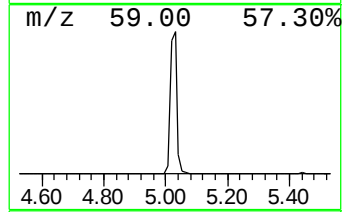
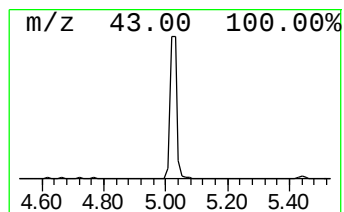
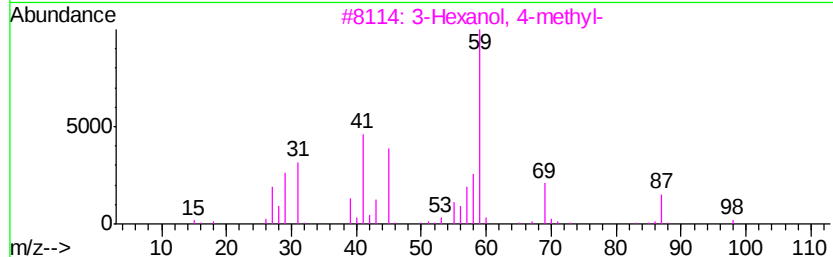
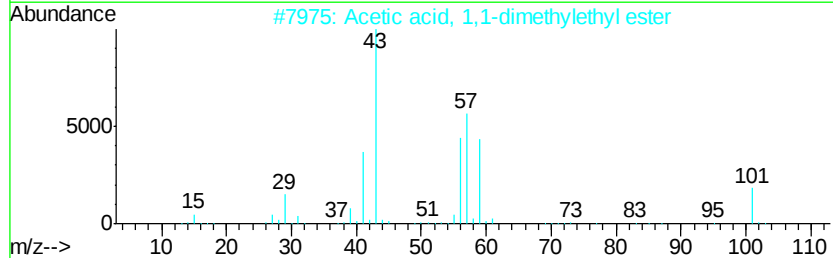
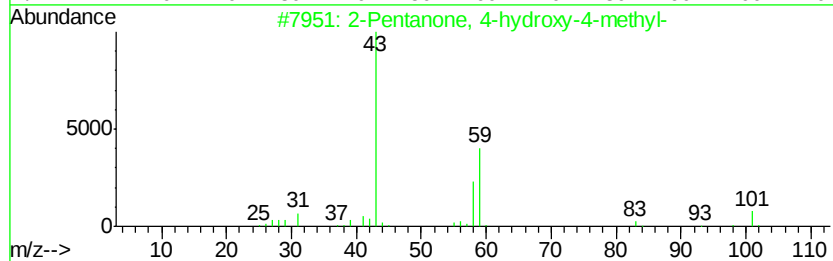
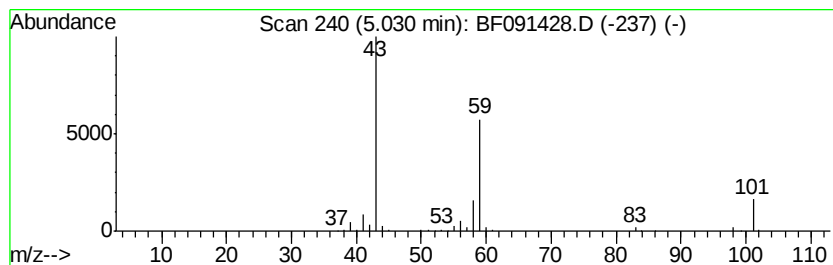
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	12.15 ng	536847	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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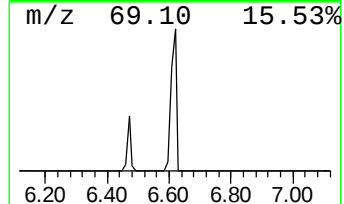
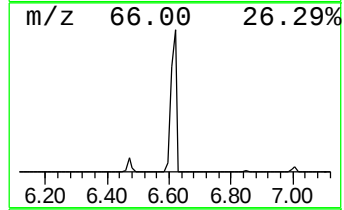
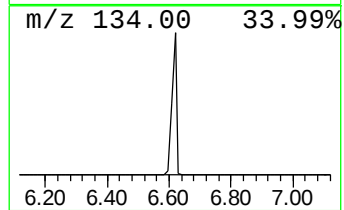
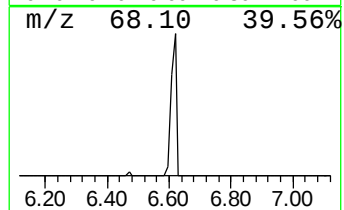
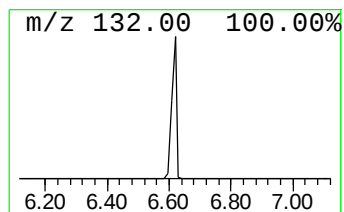
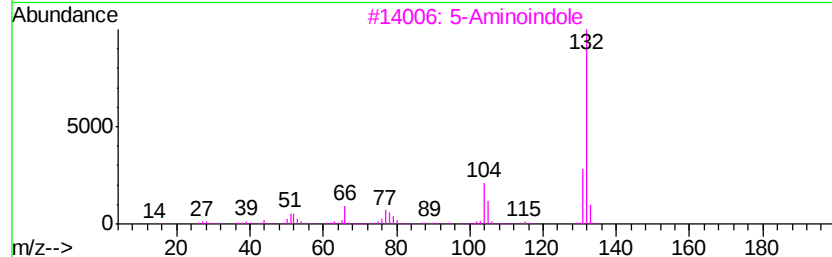
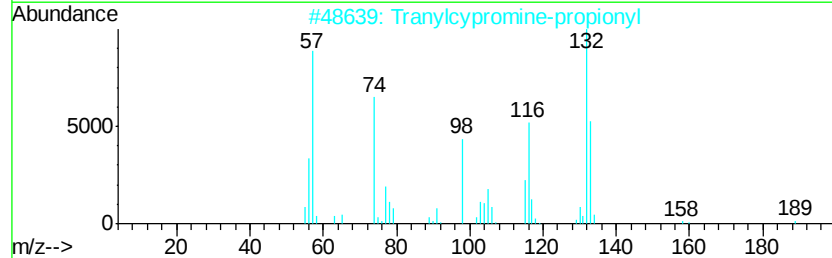
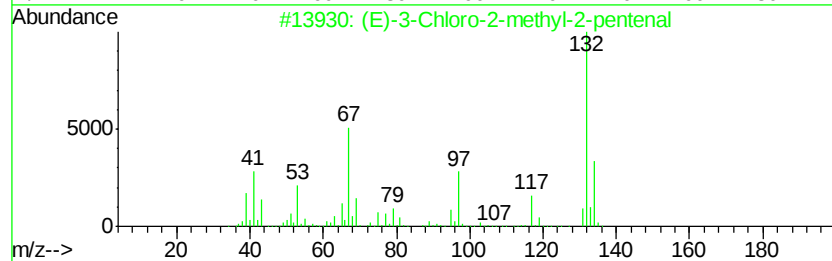
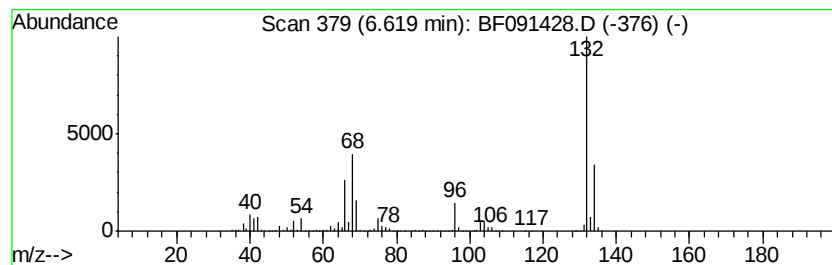
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Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	92.35 ng	4080340	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		5-Aminoindole	132	C8H8N2	005192-03-0	9
4		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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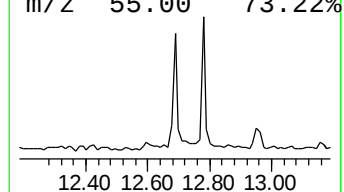
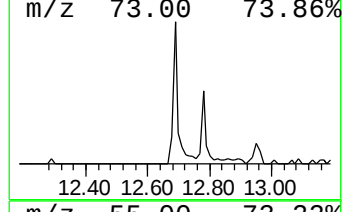
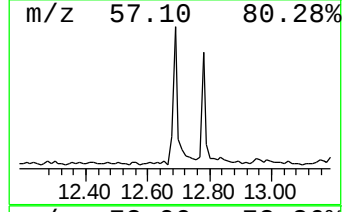
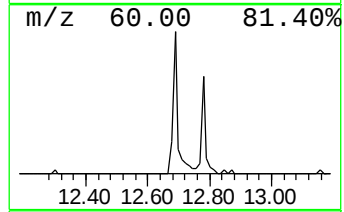
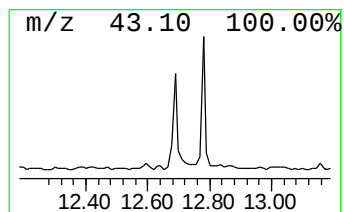
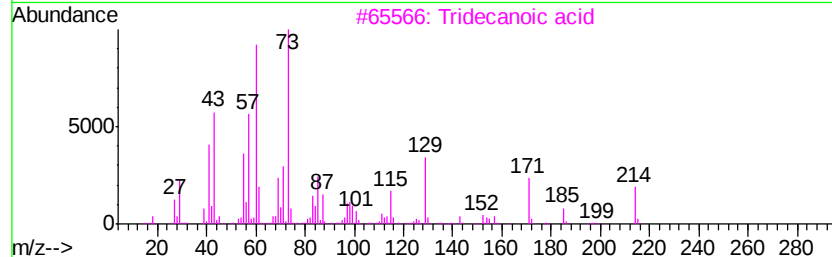
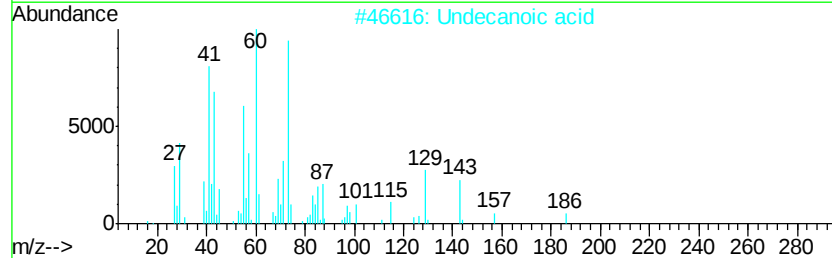
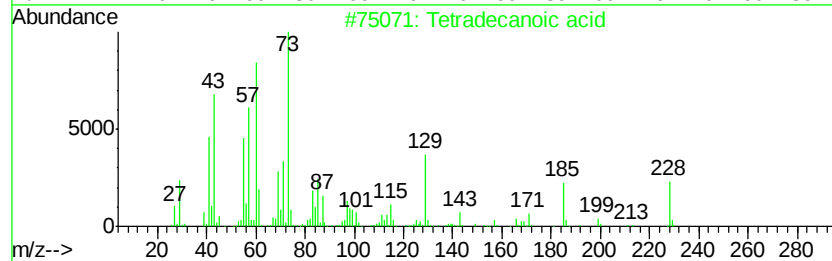
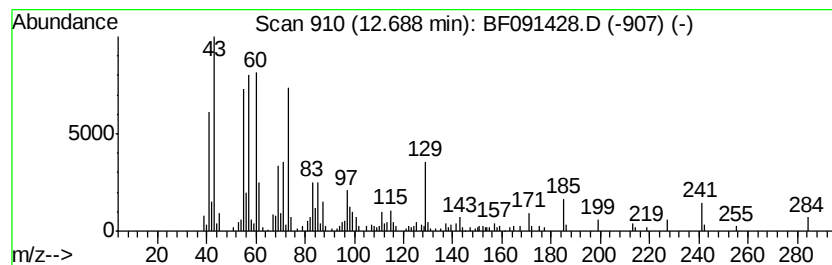
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Peak Number 4 Tetradecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.69	3.64 ng	210515	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
2	Undecanoic acid	186	C11H22O2	000112-37-8	60
3	Tridecanoic acid	214	C13H26O2	000638-53-9	59
4	n-Decanoic acid	172	C10H20O2	000334-48-5	53
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50



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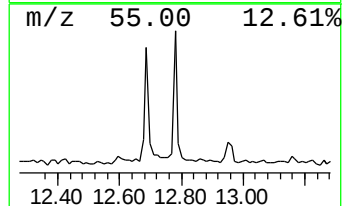
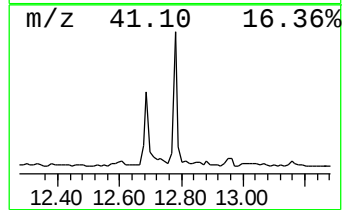
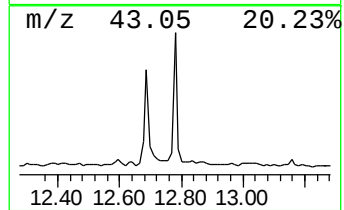
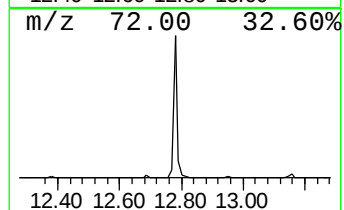
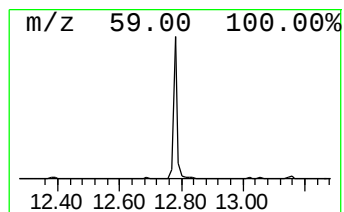
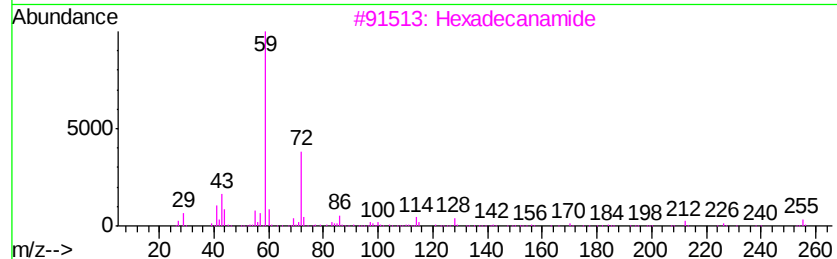
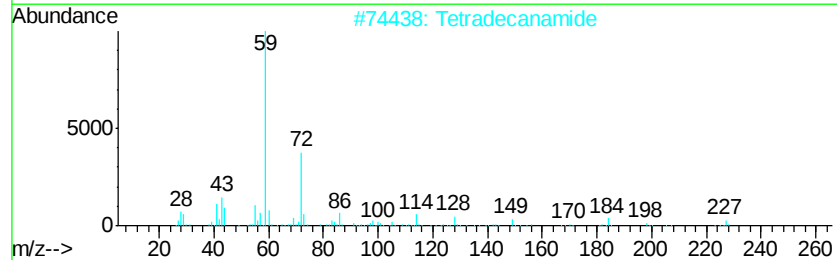
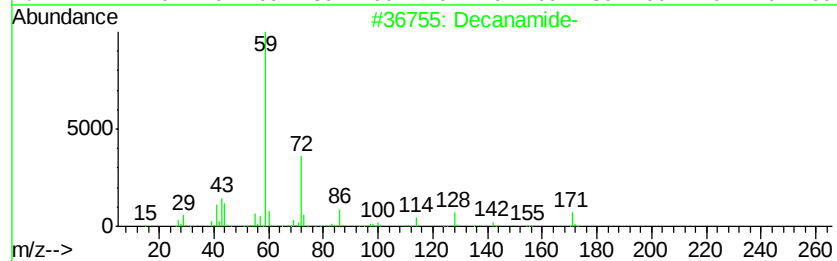
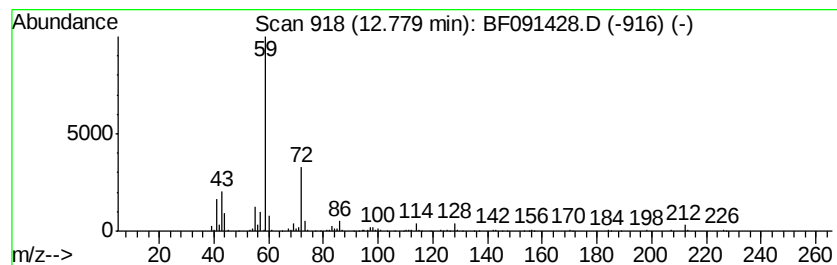
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Peak Number 5 Decanamide- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	4.60 ng	266056	Chrysene-d12	14.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanamide-		171	C10H21NO	002319-29-1	91
2	Tetradecanamide		227	C14H29NO	000638-58-4	90
3	Hexadecanamide		255	C16H33NO	000629-54-9	87
4	Dodecanamide		199	C12H25NO	001120-16-7	83
5	Undecanamide, 11-bromo-		263	C11H22BrNO	005875-26-3	78



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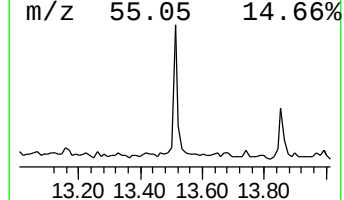
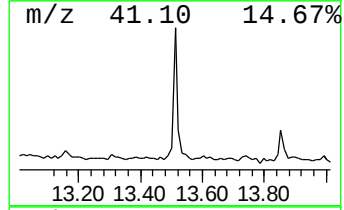
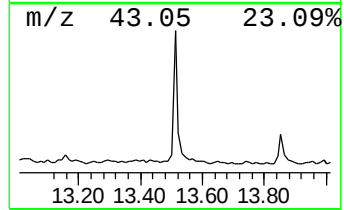
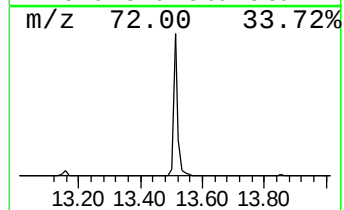
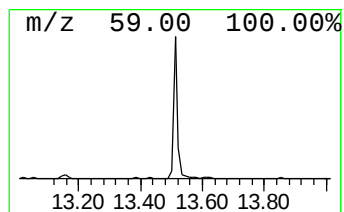
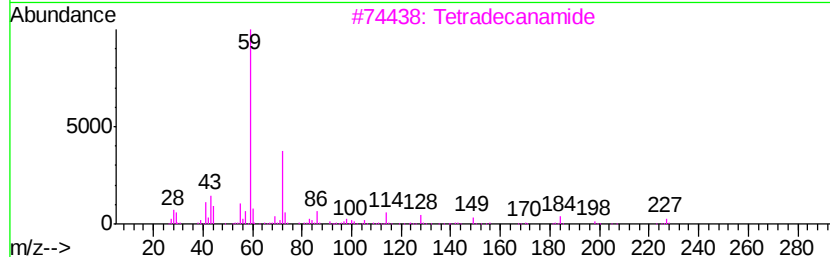
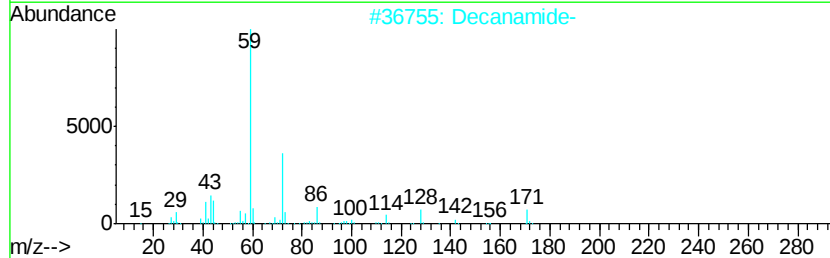
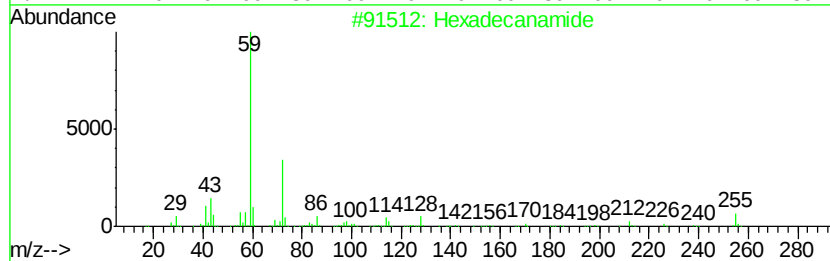
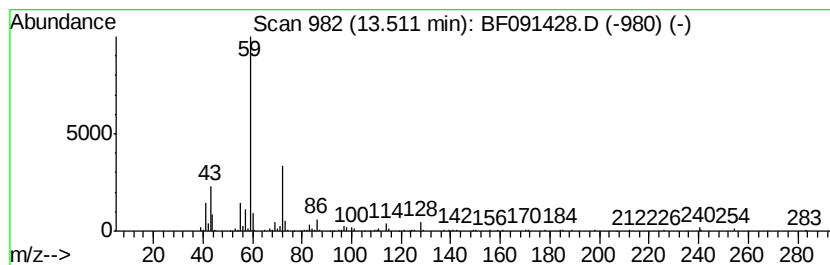
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Peak Number 6 Hexadecanamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.51	4.10 ng	237526	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanamide	255	C16H33NO	000629-54-9	90
2	Decanamide-	171	C10H21NO	002319-29-1	87
3	Tetradecanamide	227	C14H29NO	000638-58-4	80
4	Octanamide	143	C8H17NO	000629-01-6	64
5	Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.03	12.2	ng	536847	1	6.85	883626	20.0
unknown6.62	6.62	92.3	ng	4080340	1	6.85	883626	20.0
Tetradecanoic acid	12.69	3.6	ng	210515	5	14.00	1157650	20.0
Decanamide-	12.78	4.6	ng	266056	5	14.00	1157650	20.0
Hexadecanamide	13.51	4.1	ng	237526	5	14.00	1157650	20.0