

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120516\
 Data File : BF091422.D
 Acq On : 5 Dec 2016 17:14
 Operator : UM/SJ
 Sample : H5838-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-3

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	4.516	192	195	198	rVB	616241	726963	12.52%	1.980%
2	5.019	236	239	242	rBV	371168	419923	7.23%	1.144%
3	5.441	273	276	278	rBV	2136350	1926393	33.19%	5.247%
4	6.470	364	366	368	rBV	1385468	1174245	20.23%	3.198%
5	6.619	376	379	381	rBV	3285492	3789375	65.28%	10.320%
6	6.847	397	399	401	rBV	1122431	920909	15.86%	2.508%
7	7.007	410	413	415	rVB	3897959	3603151	62.07%	9.813%
8	7.407	445	448	451	rVB	2196717	2921811	50.33%	7.958%
9	8.127	509	511	514	rBV	801106	979506	16.87%	2.668%
10	9.213	603	606	608	rBV	5368447	5013823	86.37%	13.655%
11	9.888	662	665	667	rBV	1521069	1351492	23.28%	3.681%
12	10.676	731	734	736	rBV	3780932	4129469	71.14%	11.247%
13	11.362	792	794	797	rBV	1274335	1406569	24.23%	3.831%
14	11.899	839	841	843	rBV	182680	176569	3.04%	0.481%
15	12.688	908	910	916	rBV	155209	210457	3.63%	0.573%
16	12.962	930	934	936	rBV	4072161	5804941	100.00%	15.810%
17	13.854	1010	1012	1016	rBV	59936	71707	1.24%	0.195%
18	13.991	1022	1024	1027	rBV	894383	1249694	21.53%	3.404%
19	15.420	1146	1149	1152	rBV	648415	840609	14.48%	2.289%

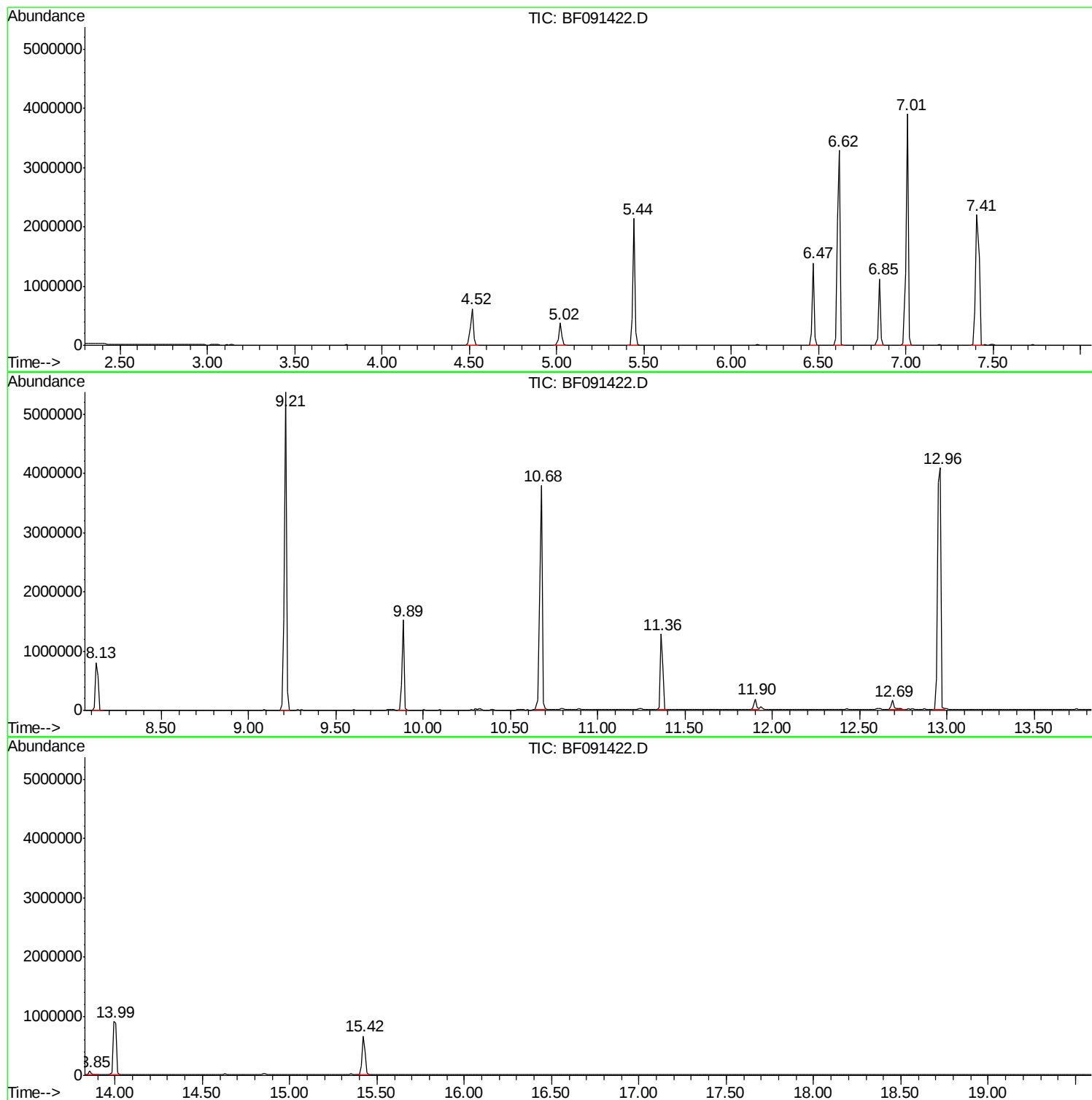
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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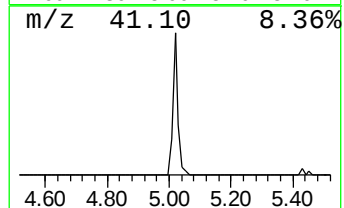
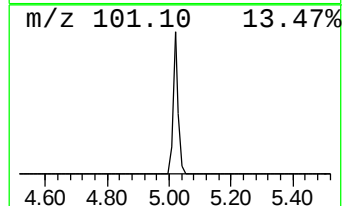
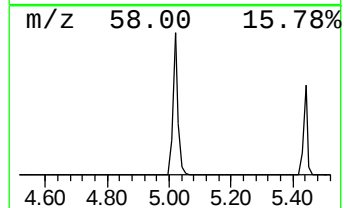
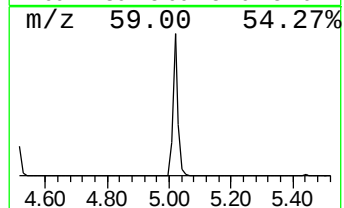
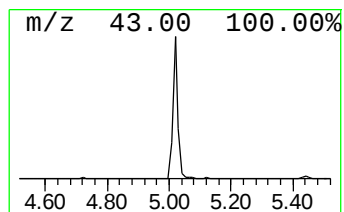
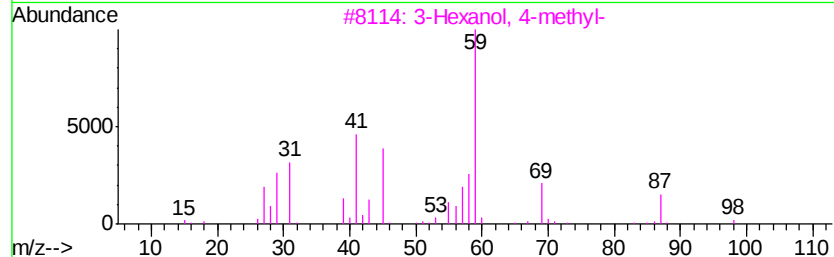
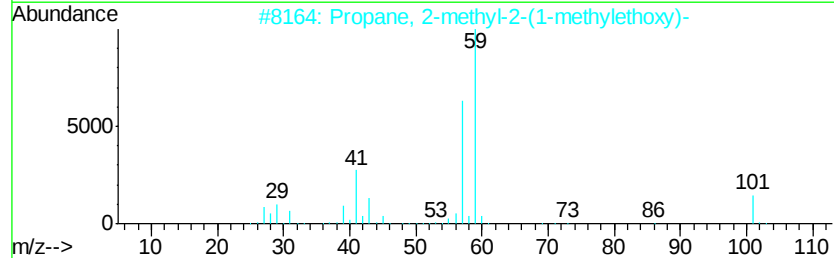
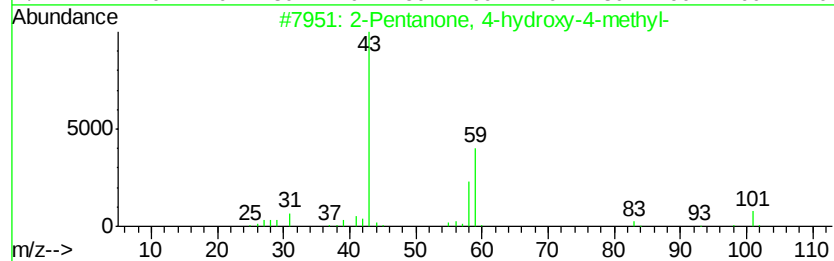
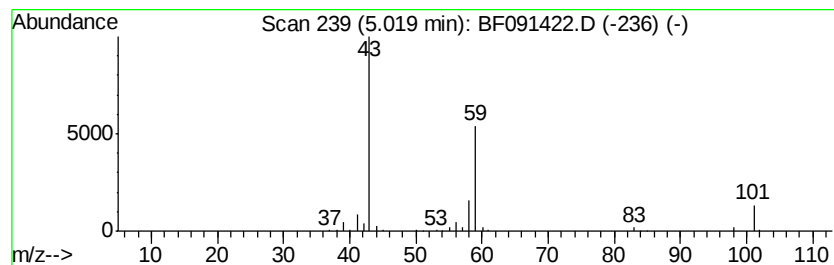
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	9.12 ng	419923	1,4-Dichlorobenzene-d4	6.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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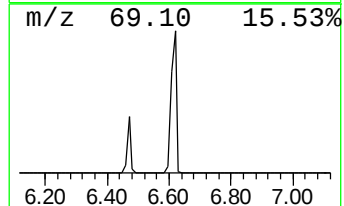
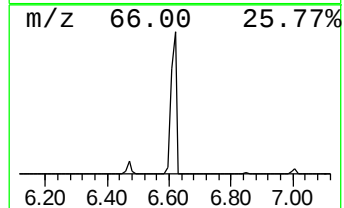
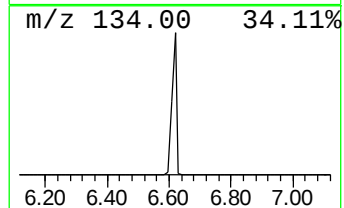
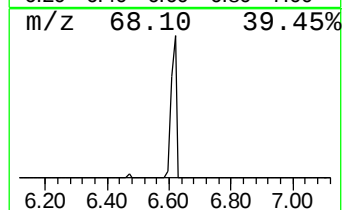
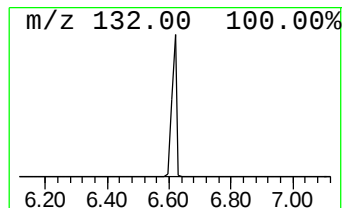
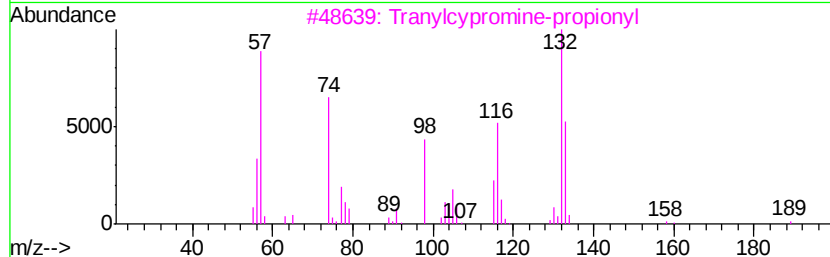
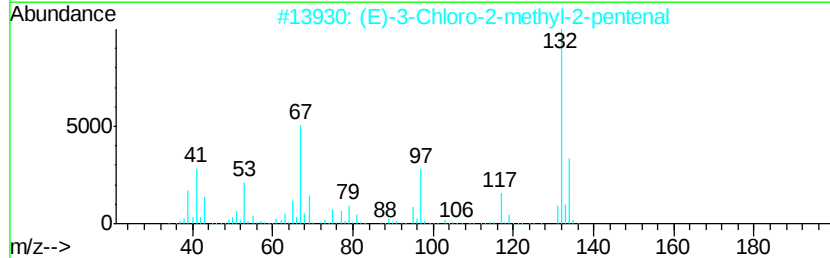
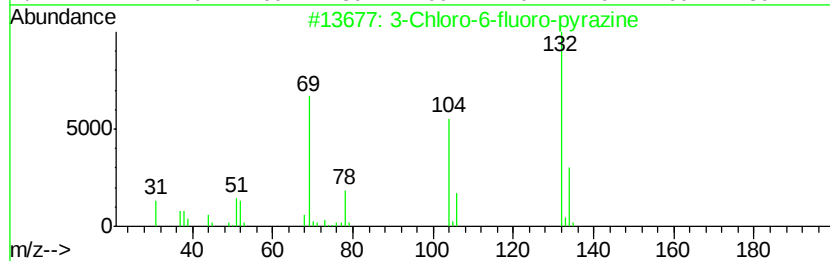
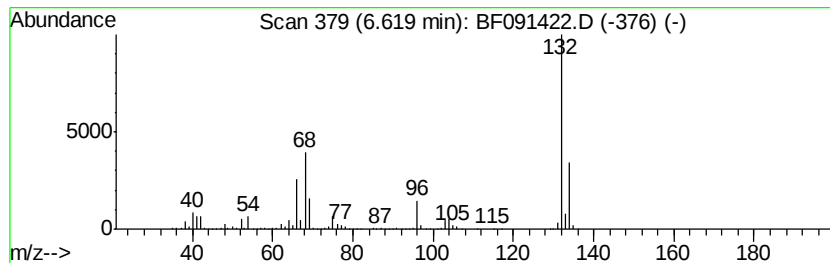
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Peak Number 3 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	82.30 ng	3789380	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		5-Aminoindole	132	C8H8N2	005192-03-0	9
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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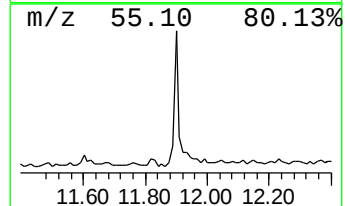
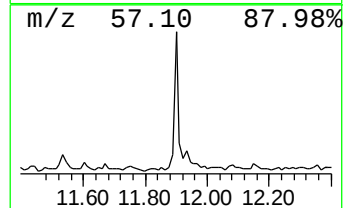
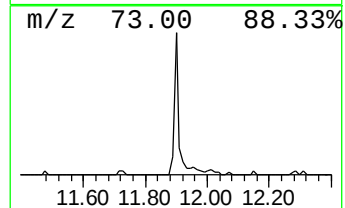
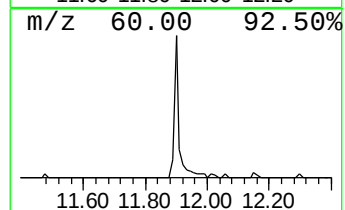
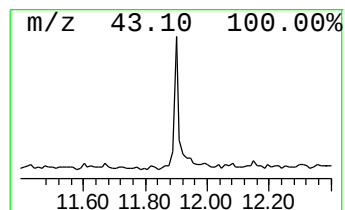
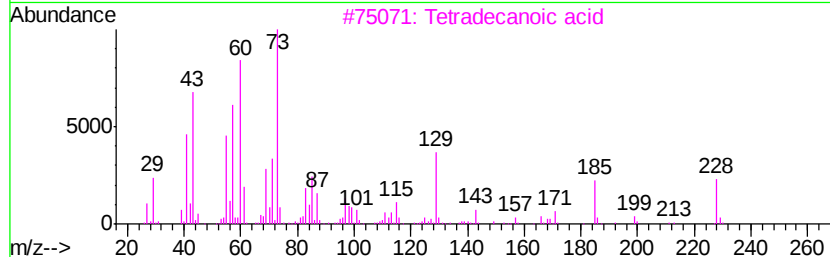
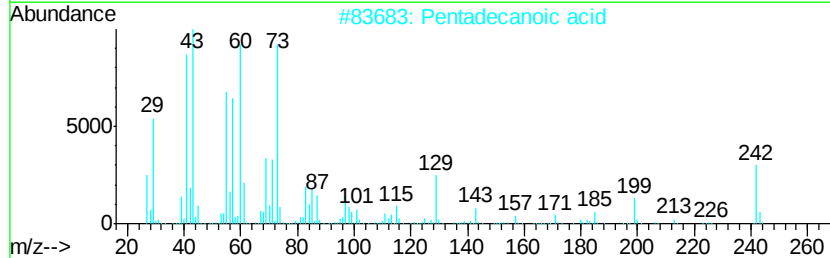
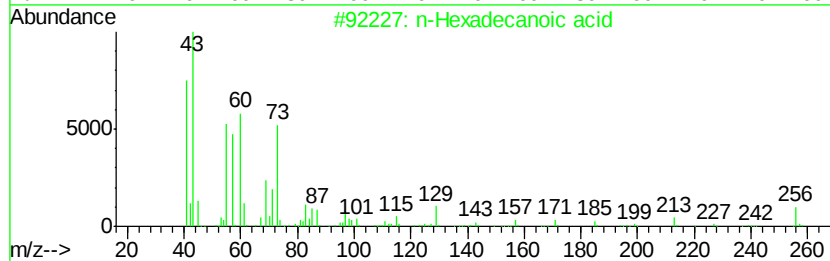
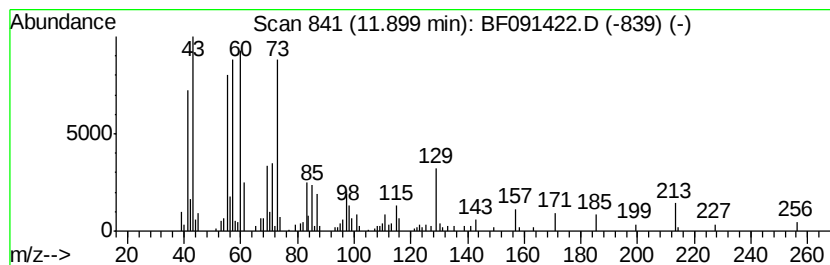
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	2.51 ng	176569	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Undecanoic acid	186	C11H22O2	000112-37-8	59
5	Tridecanoic acid	214	C13H26O2	000638-53-9	59



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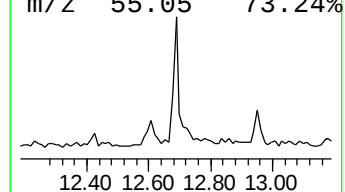
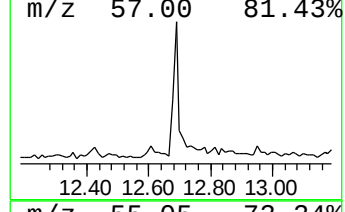
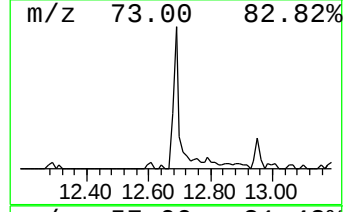
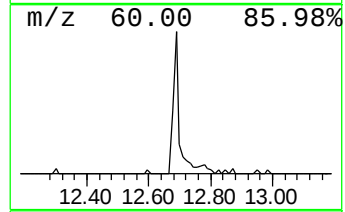
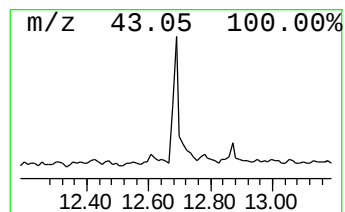
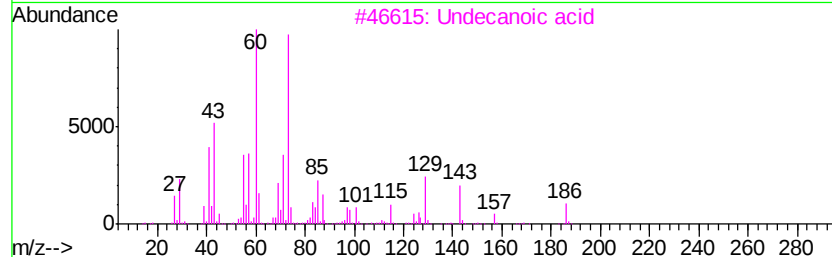
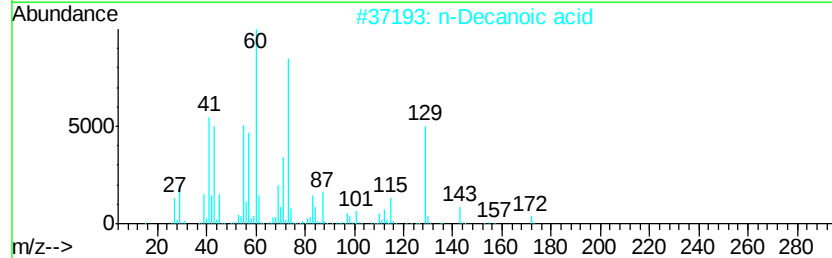
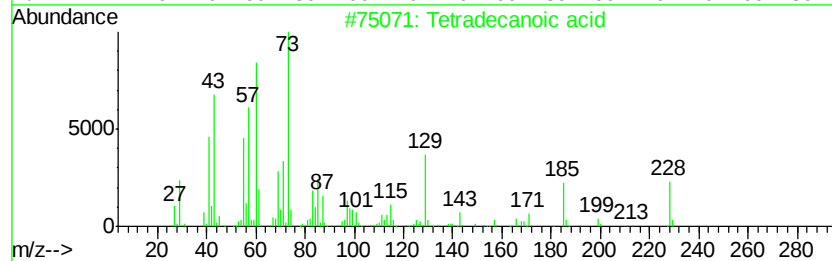
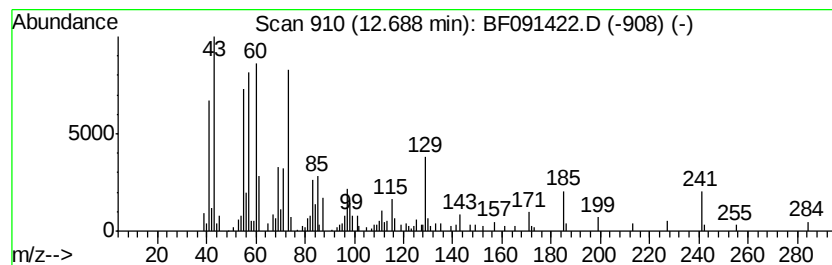
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Peak Number 6 Tetradecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.69	3.37 ng	210457	Chrysene-d12		14.00
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
2	n-Decanoic acid	172	C10H20O2	000334-48-5	55
3	Undecanoic acid	186	C11H22O2	000112-37-8	53
4	Tridecanoic acid	214	C13H26O2	000638-53-9	53
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.02	9.1 ng		419923	1	6.85	920909	20.0
unknown6.62	6.62	82.3 ng		3789380	1	6.85	920909	20.0
n-Hexadecanoic acid	11.90	2.5 ng		176569	4	11.36	1406570	20.0
Tetradecanoic acid	12.69	3.4 ng		210457	5	14.00	1249690	20.0