

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080417\
Data File : BF097360.D
Acq On : 4 Aug 2017 17:17
Operator : SJ/JU
Sample : I4535-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TRC-MW-101D

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-BF072517.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	1.857	8	12	26	rVB	508701	722606	22.26%	2.826%
2	1.957	26	29	53	rVB	186699	351156	10.82%	1.374%
3	3.975	367	372	381	rBV	143648	226373	6.97%	0.885%
4	4.569	470	473	488	rBV	104255	181530	5.59%	0.710%
5	5.034	549	552	574	rBV	1474306	1811968	55.82%	7.087%
6	6.104	731	734	748	rBV	966991	1173688	36.16%	4.591%
7	6.210	748	752	763	rVB	2664859	2761855	85.08%	10.803%
8	6.439	787	791	799	rBV	716286	738226	22.74%	2.887%
9	6.592	813	817	835	rBV	2426479	2402803	74.02%	9.398%
10	7.010	883	888	891	rBV	2049136	2137815	65.86%	8.362%
11	7.722	1005	1009	1026	rVB	982245	962178	29.64%	3.763%
12	8.798	1186	1192	1195	rBV	3078571	3246157	100.00%	12.697%
13	9.198	1256	1260	1265	rBV	50758	45086	1.39%	0.176%
14	9.457	1300	1304	1314	rVB	1042283	1023923	31.54%	4.005%
15	10.251	1434	1439	1448	rBV	1724921	1922888	59.24%	7.521%
16	10.933	1551	1555	1562	rBV	1051171	962946	29.66%	3.766%
17	11.486	1646	1649	1660	rBV2	87256	113942	3.51%	0.446%
18	12.269	1778	1782	1791	rBV2	67005	103462	3.19%	0.405%
19	12.516	1819	1824	1827	rBV	2514176	3027210	93.26%	11.841%
20	13.551	1996	2000	2009	rBV	932023	897221	27.64%	3.509%
21	14.398	2139	2144	2149	rBV	53650	52529	1.62%	0.205%
22	14.886	2223	2227	2232	rBV	588257	700863	21.59%	2.741%

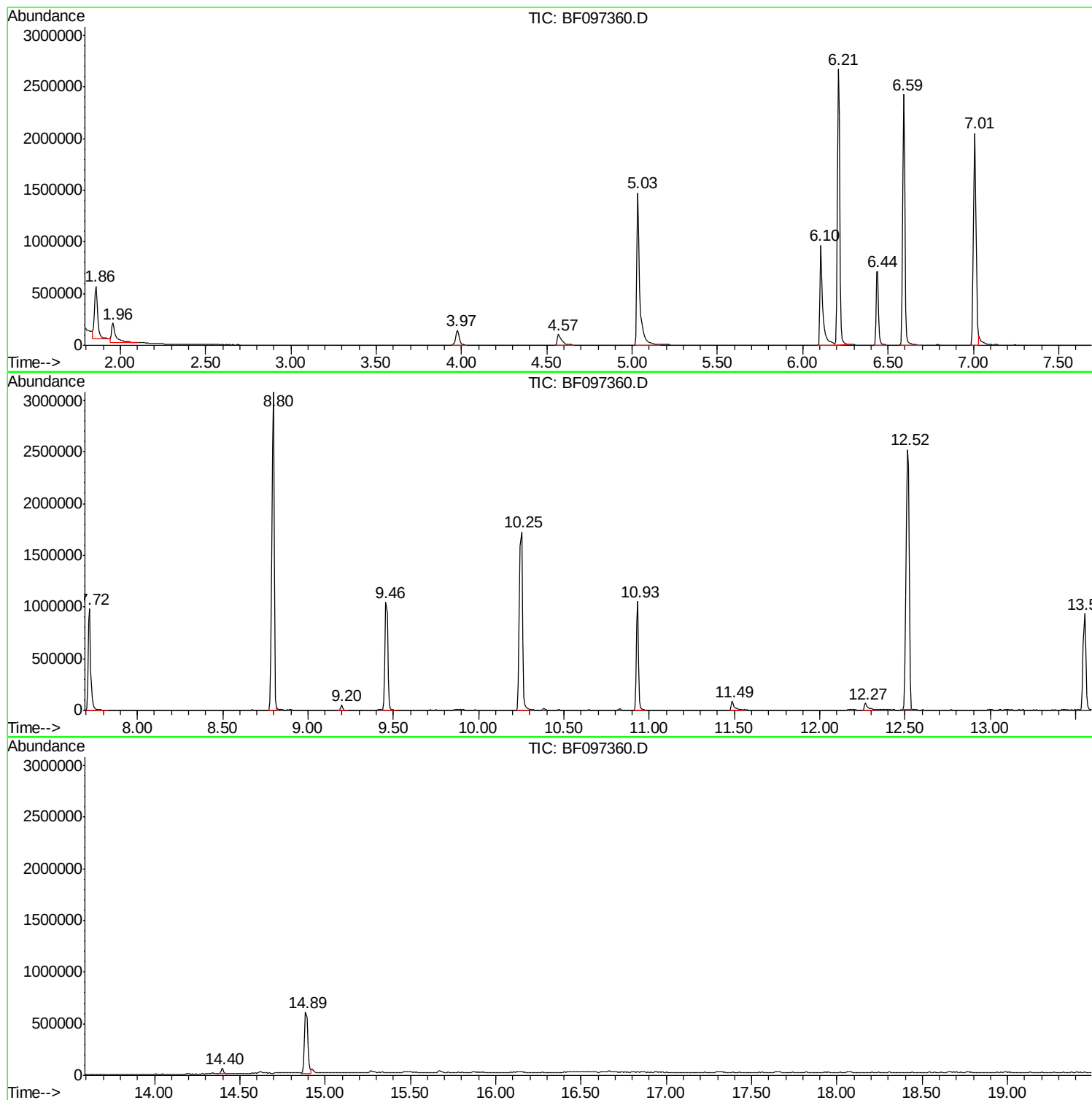
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampled :
TRC-MW-101D

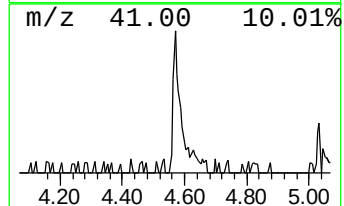
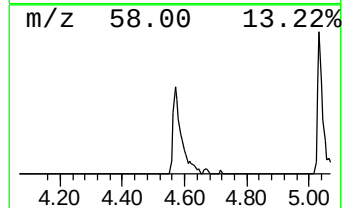
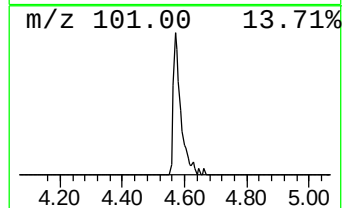
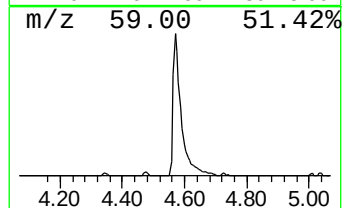
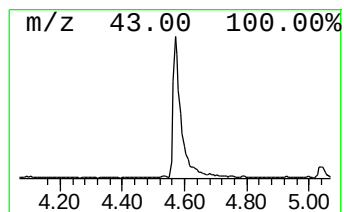
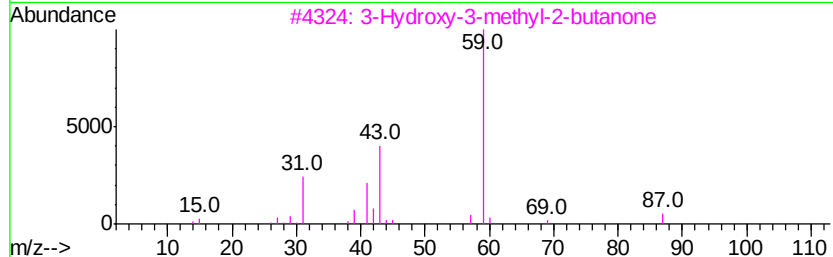
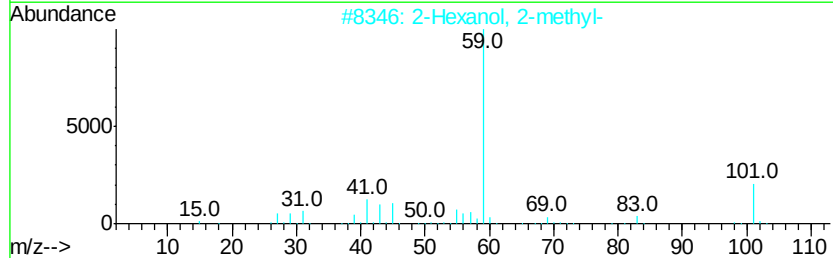
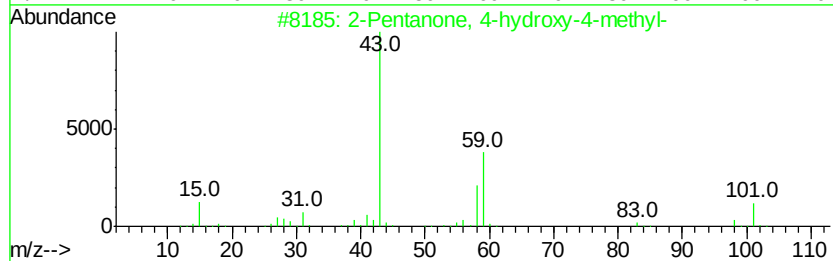
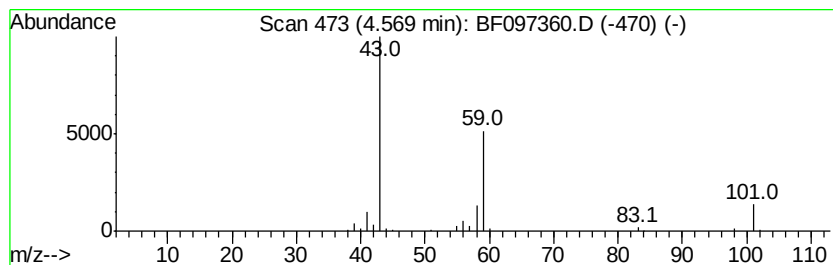
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	4.92 ng	181530	1,4-Dichlorobenzene-d4	6.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Silane, trimethyl-	74	C3H10Si	000993-07-7	9



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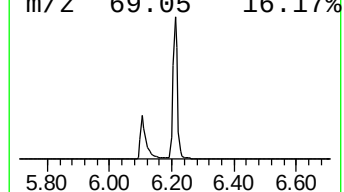
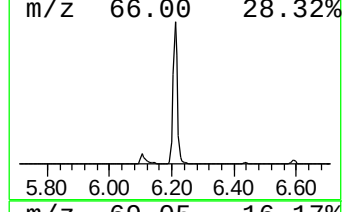
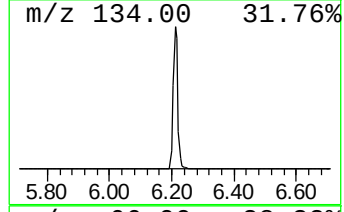
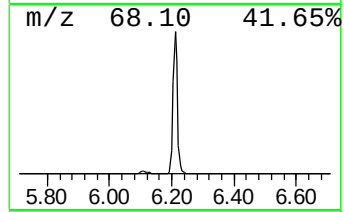
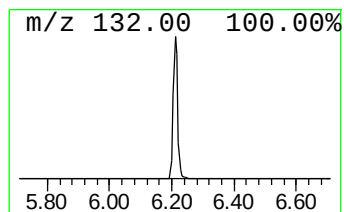
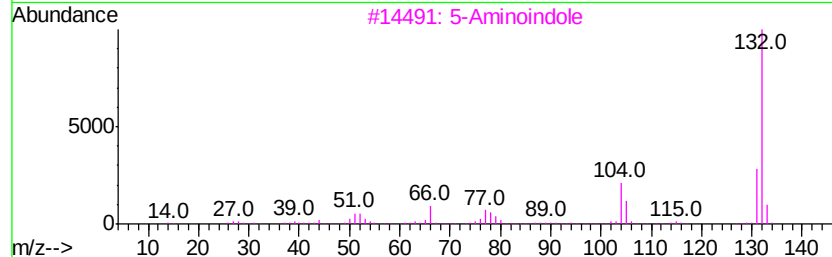
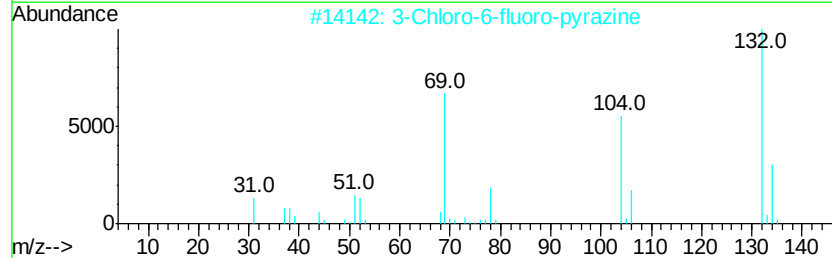
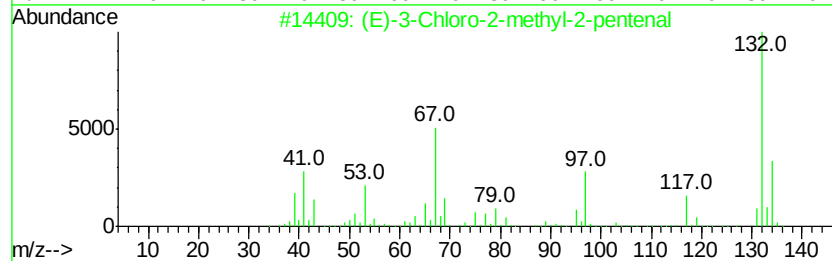
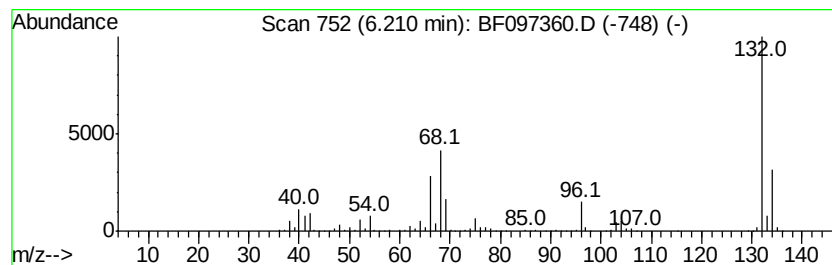
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Peak Number 4 unknown6.21 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.21	74.82 ng	2761860	1,4-Dichlorobenzene-d4	6.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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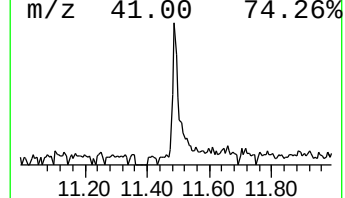
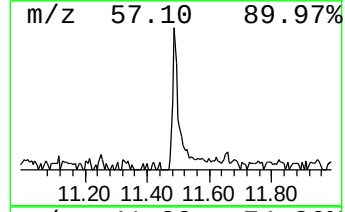
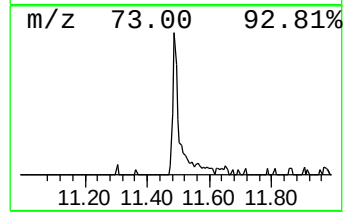
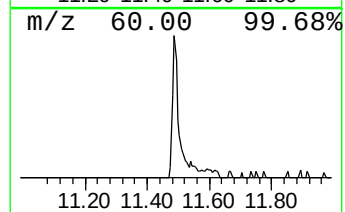
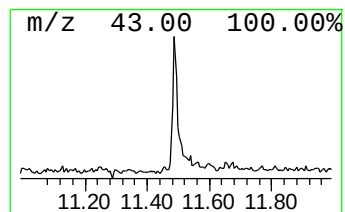
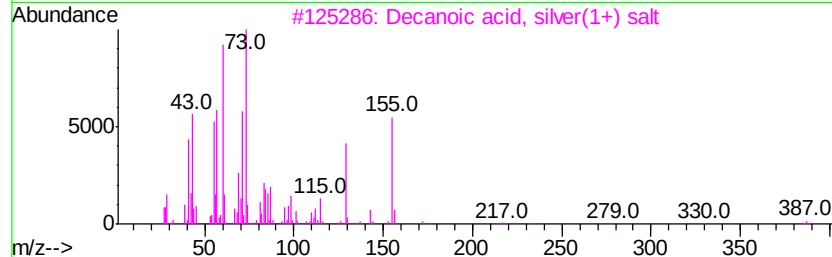
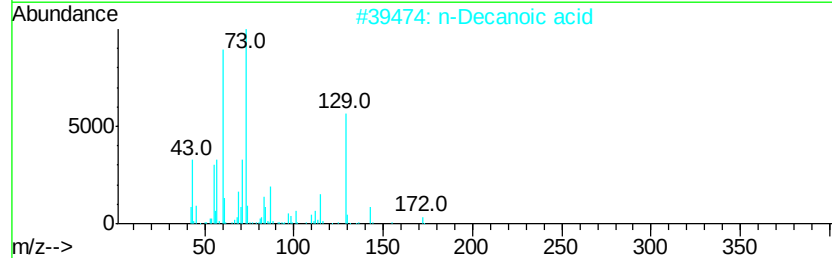
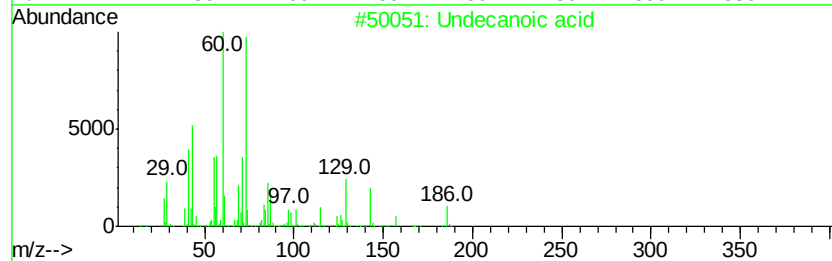
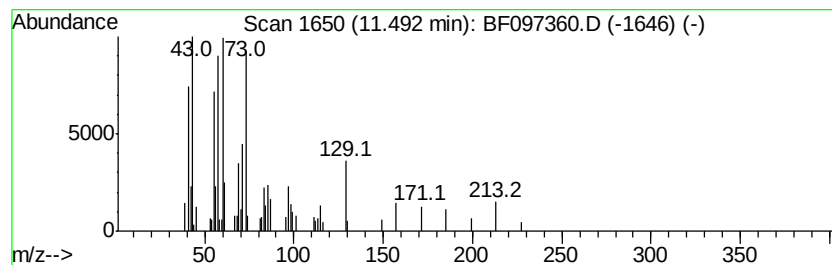
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Peak Number 6 Undecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.49	2.37 ng	113942	Phenanthrene-d10	10.93	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	86
2	n-Decanoic acid	172	C10H20O2	000334-48-5	64
3	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	47
4	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	43
5	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	22



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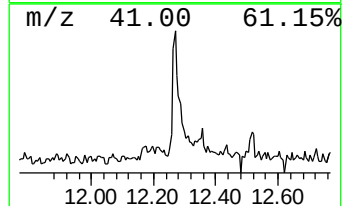
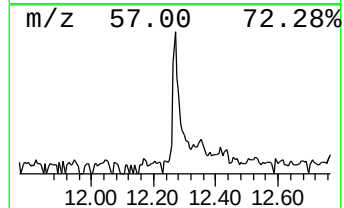
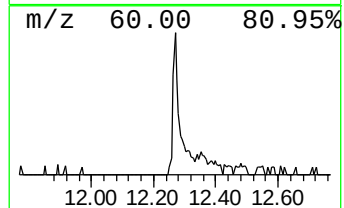
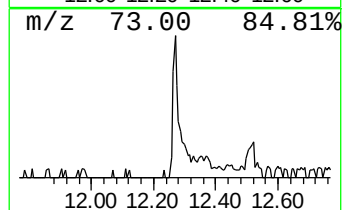
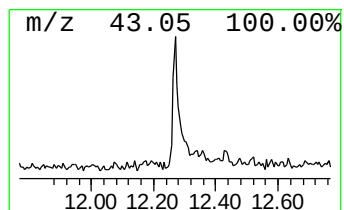
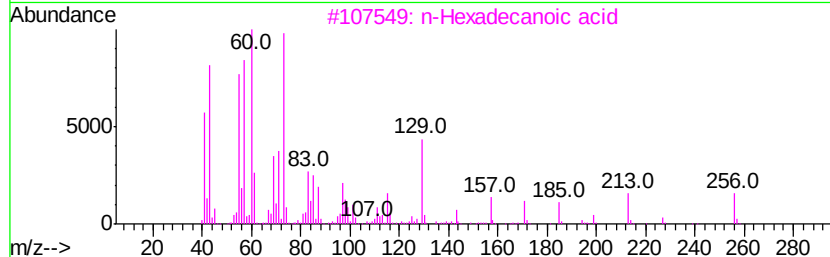
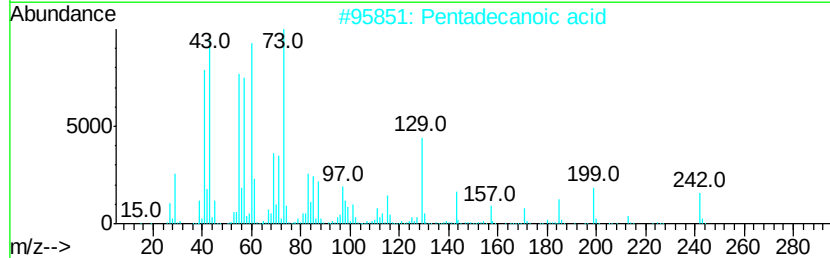
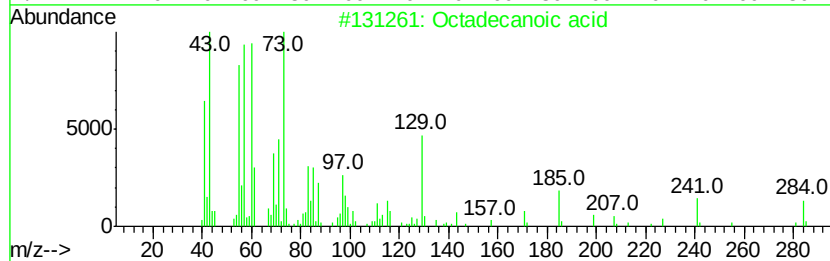
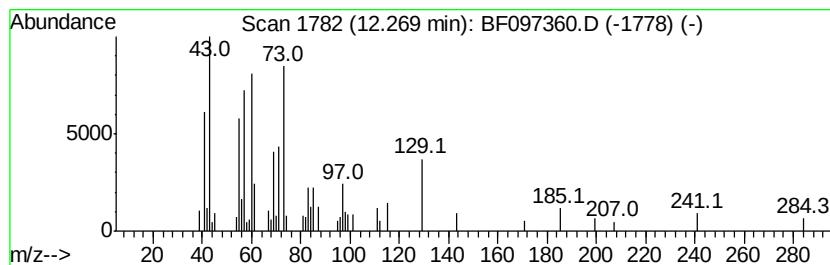
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.27	2.31 ng	103462	Chrysene-d12	13.55

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	96
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	78
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
4		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	72
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.57	4.9	ng	181530	1	6.44	738226	20.0
unknown6.21	6.21	74.8	ng	2761860	1	6.44	738226	20.0
Undecanoic acid	11.49	2.4	ng	113942	4	10.93	962946	20.0
Octadecanoic acid	12.27	2.3	ng	103462	5	13.55	897221	20.0