

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012918\
 Data File : BF102608.D
 Acq On : 29 Jan 2018 20:22
 Operator : SJ/JU
 Sample : J1344-06
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 8-SAN-4-EW(4-5)

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-BF012218.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	4.928	479	483	491	rBV	83548	130091	2.92%	0.333%
2	5.334	547	552	569	rBV	3713090	4147745	92.97%	10.628%
3	6.363	722	727	743	rBV	3457256	4376055	98.09%	11.213%
4	6.486	743	748	751	rBV	4259072	4122122	92.40%	10.563%
5	6.551	756	759	769	rVB	116551	149216	3.34%	0.382%
6	6.710	783	786	793	rBV	1098712	959252	21.50%	2.458%
7	6.869	809	813	816	rBV	3562357	3213756	72.04%	8.235%
8	7.286	878	884	894	rBV	2407472	2784885	62.42%	7.136%
9	7.998	1001	1005	1027	rVB	1300497	1368587	30.68%	3.507%
10	9.075	1183	1188	1191	rBV	4546743	4461170	100.00%	11.431%
11	9.469	1251	1255	1266	rBV	238547	256197	5.74%	0.656%
12	9.751	1298	1303	1314	rBV	1490108	1490113	33.40%	3.818%
13	10.174	1372	1375	1378	rVB	78364	65549	1.47%	0.168%
14	10.545	1434	1438	1452	rBV	2450837	2570359	57.62%	6.586%
15	10.645	1452	1455	1459	rBV	100859	92006	2.06%	0.236%
16	11.233	1552	1555	1566	rBV	1423490	1496328	33.54%	3.834%
17	12.821	1820	1825	1829	rBV	3716245	4168742	93.45%	10.682%
18	13.709	1973	1976	1987	rBV	422265	635057	14.24%	1.627%
19	13.880	2001	2005	2014	rBV	1177977	1219309	27.33%	3.124%
20	13.962	2016	2019	2023	rBV	73462	67189	1.51%	0.172%
21	14.615	2127	2130	2137	rBV2	143613	182892	4.10%	0.469%
22	15.309	2243	2248	2256	rBV	773564	1068657	23.95%	2.738%

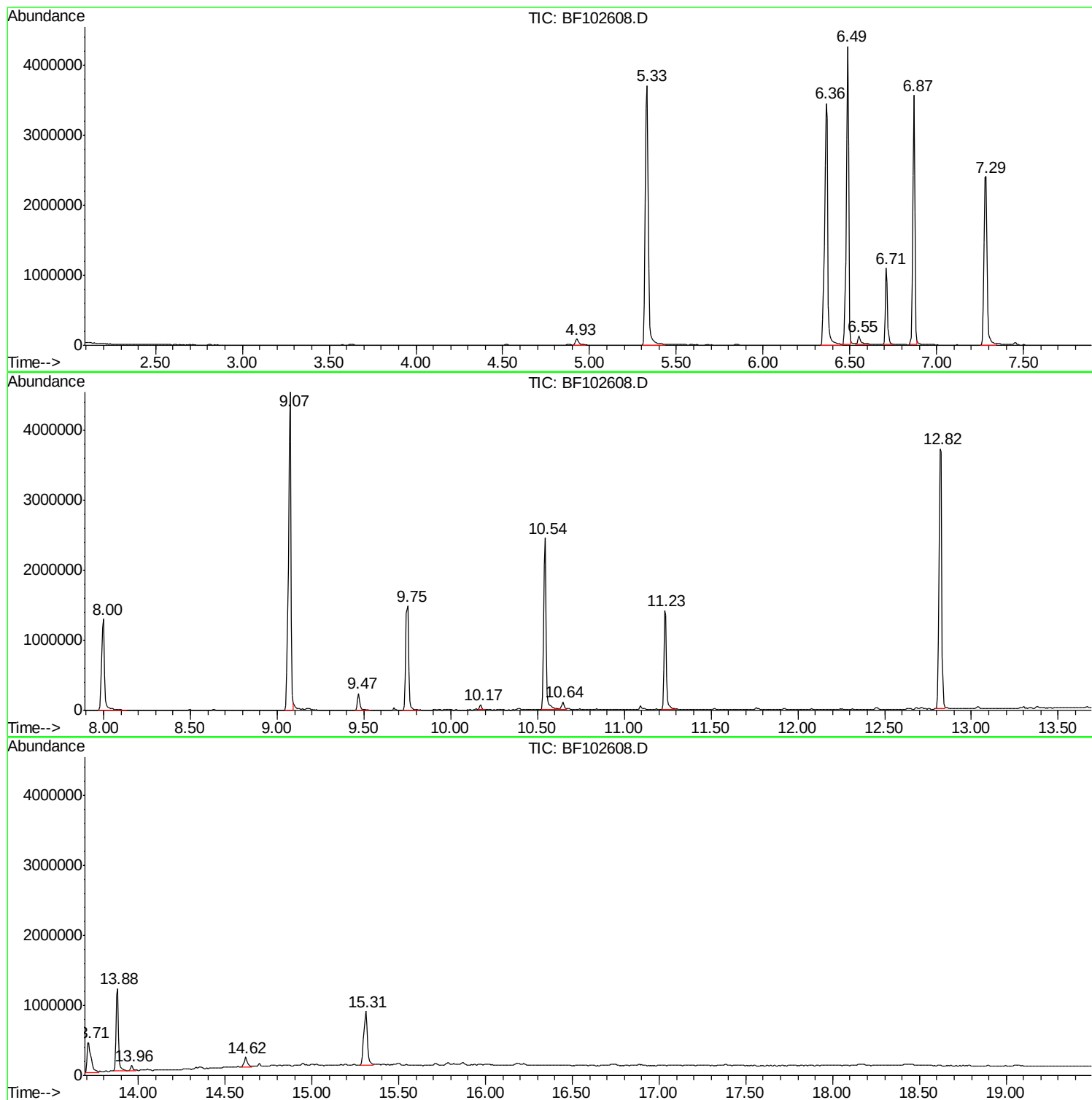
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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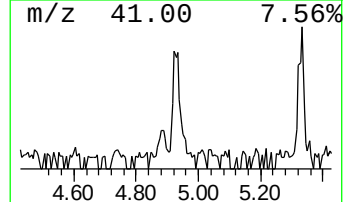
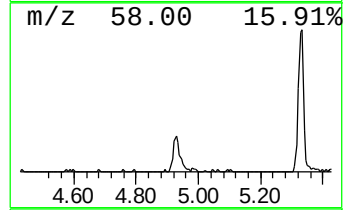
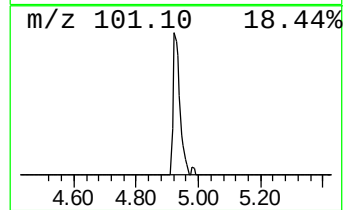
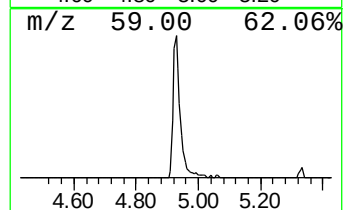
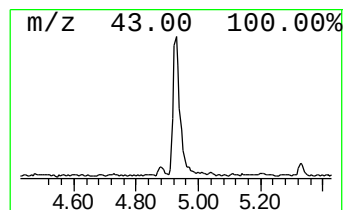
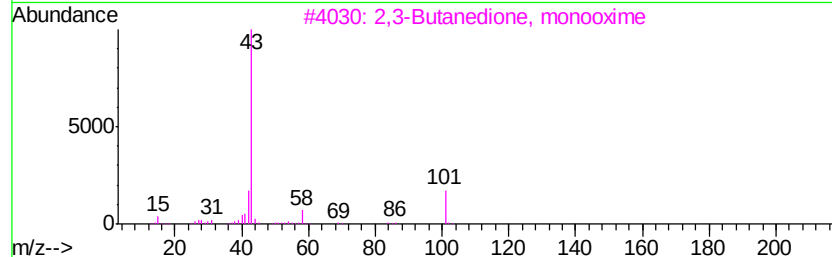
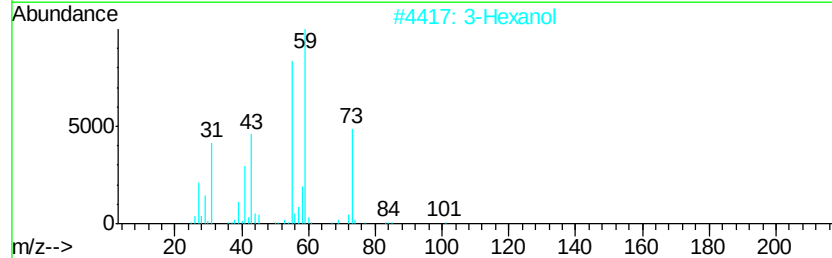
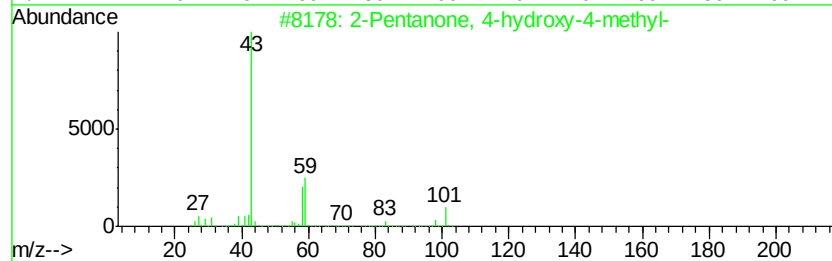
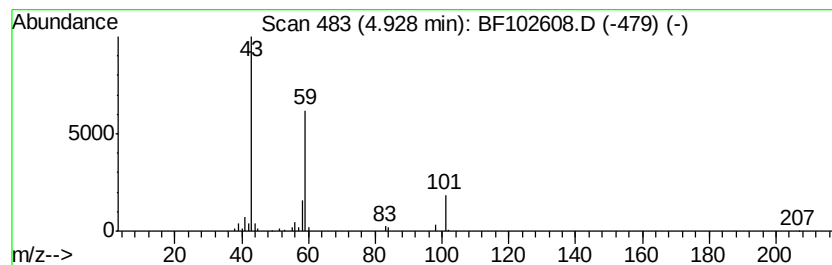
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	2.71 ng	130091	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			3-Hexanol	102	C6H14O	000623-37-0	36
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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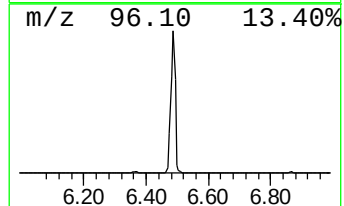
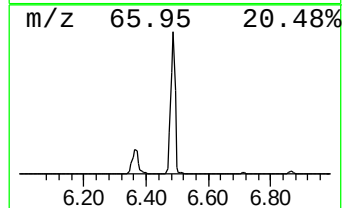
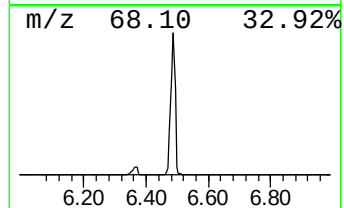
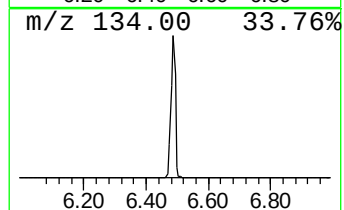
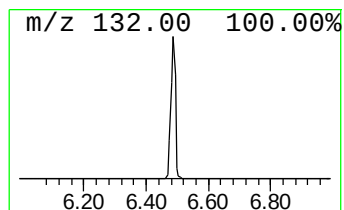
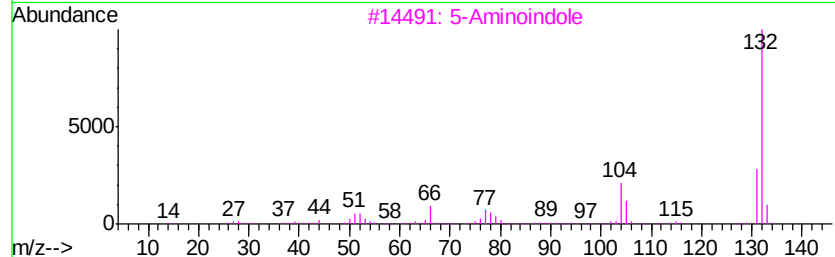
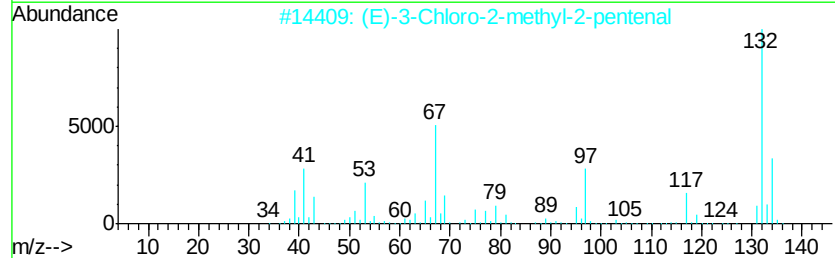
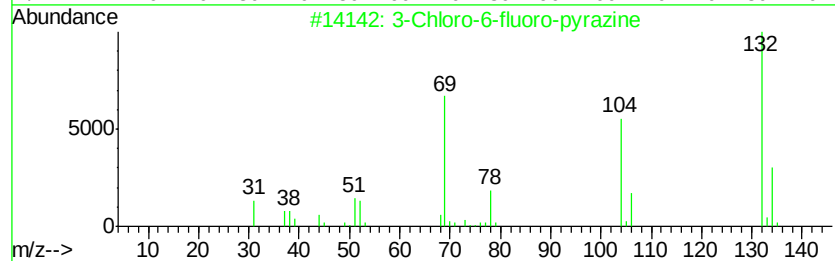
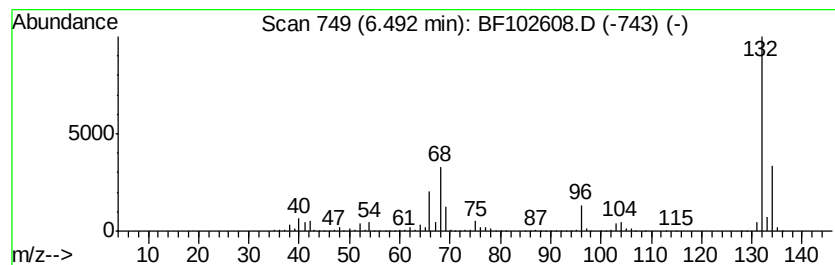
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Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	85.94 ng	4122120	1,4-Dichlorobenzene-d4	6.71

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	16
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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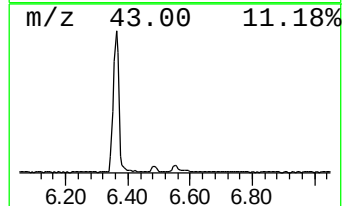
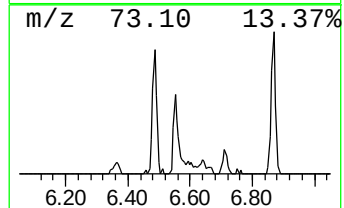
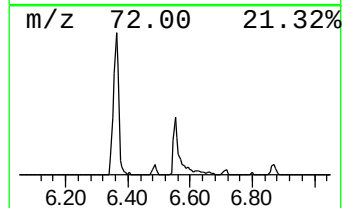
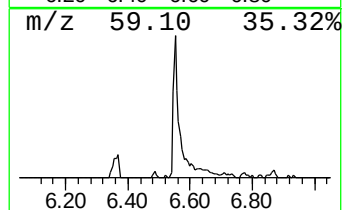
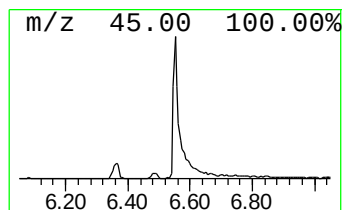
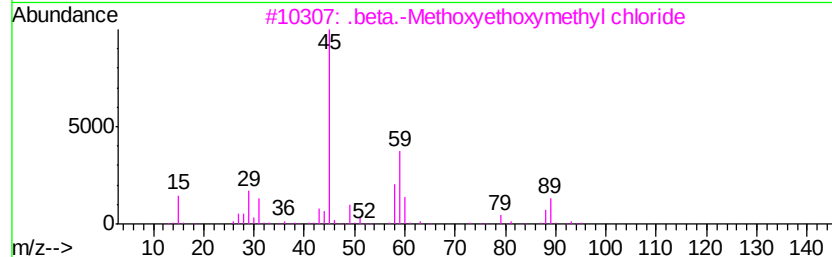
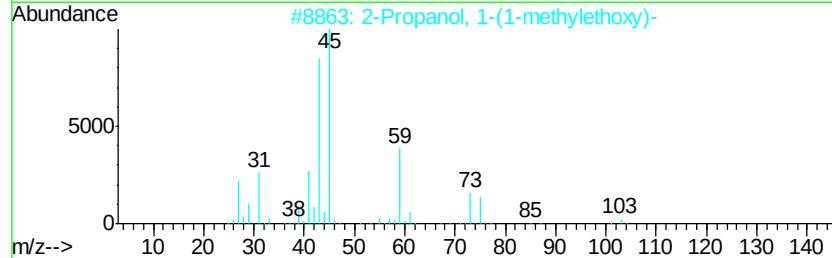
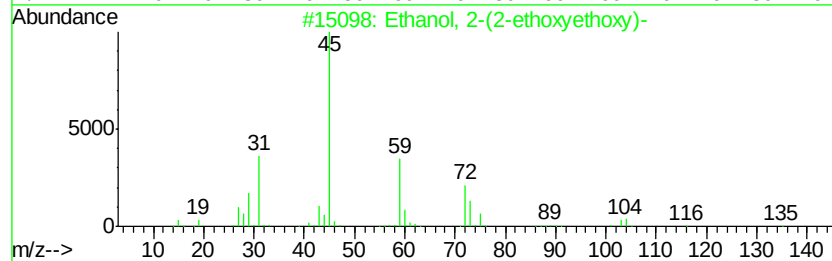
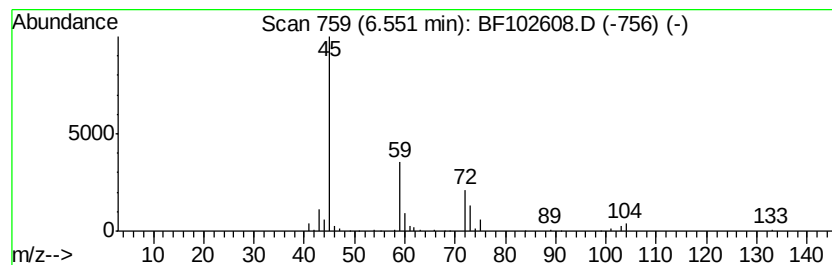
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Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.55	3.11 ng	149216	1,4-Dichlorobenzene-d4	6.71	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38
3	.beta.-Methoxyethoxymethyl chloride	124	C4H9ClO2	003970-21-6	36
4	Diethyl carbitol	162	C8H18O3	000112-36-7	12
5	2-Hydroxyethyl vinyl sulfide	104	C4H8OS	003090-56-0	9



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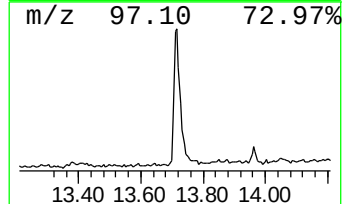
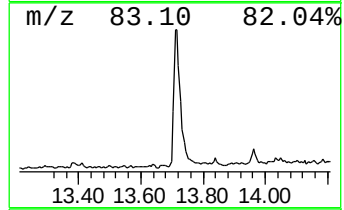
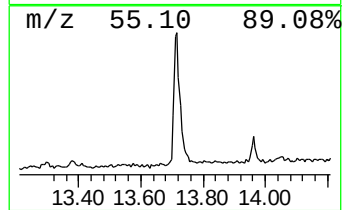
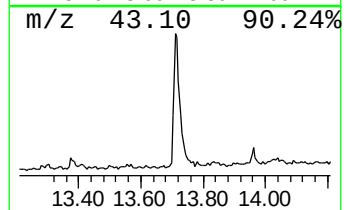
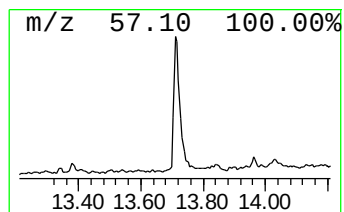
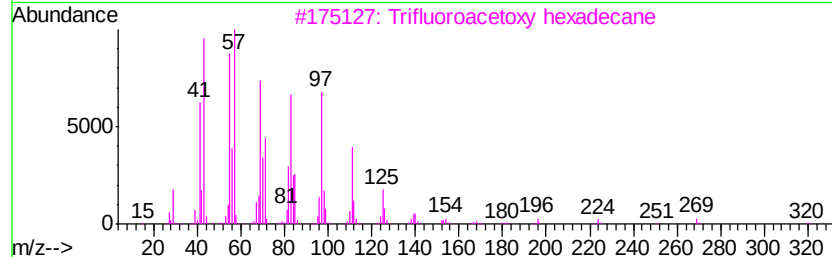
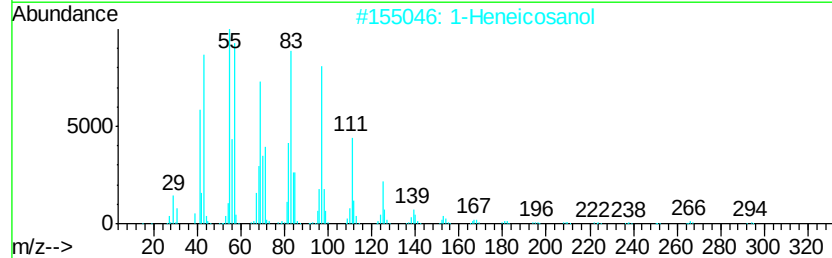
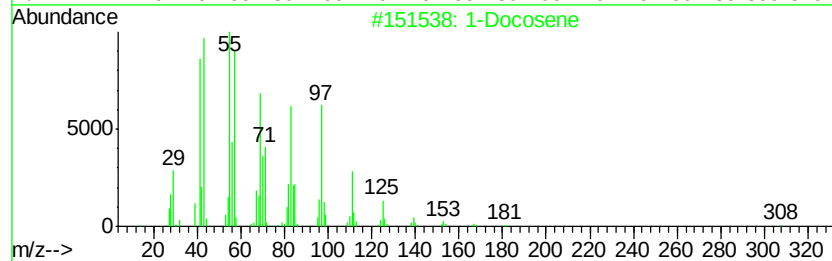
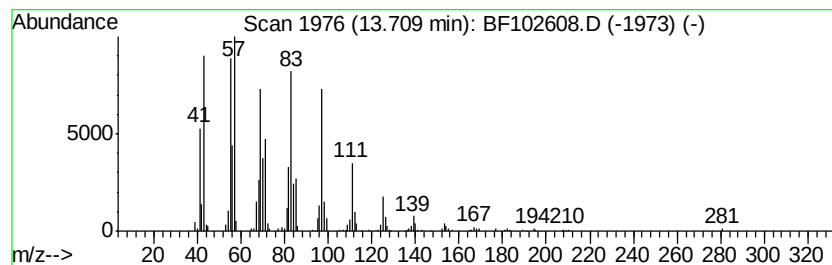
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	10.42 ng	635057	Chrysene-d12	13.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	94
2		1-Heneicosanol	312	C21H44O	015594-90-8	93
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
4		1-Octadecanol	270	C18H38O	000112-92-5	93
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93



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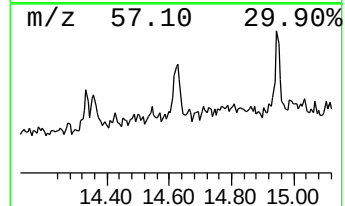
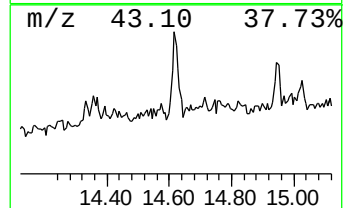
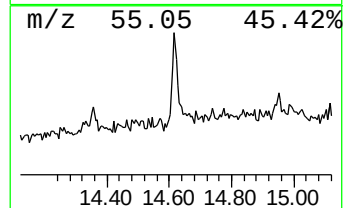
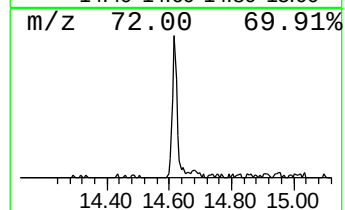
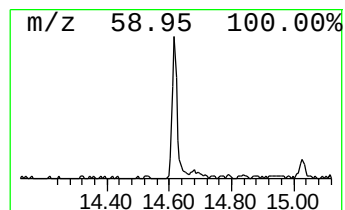
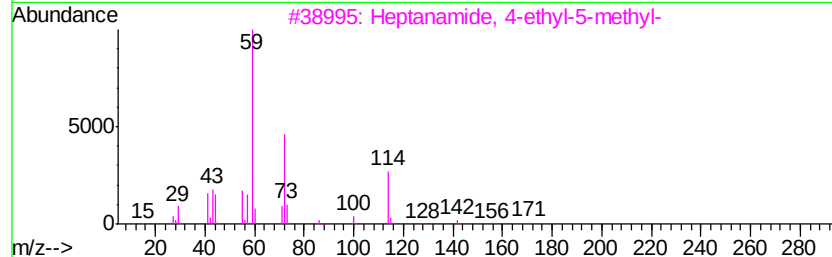
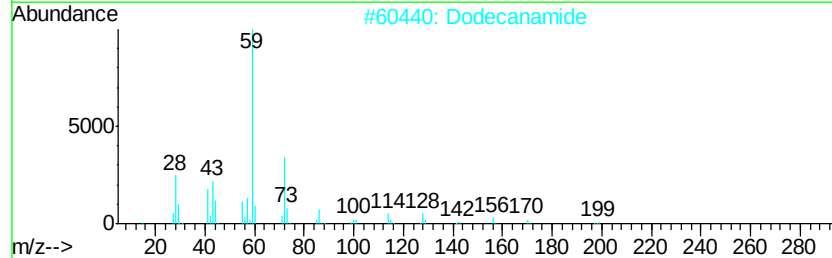
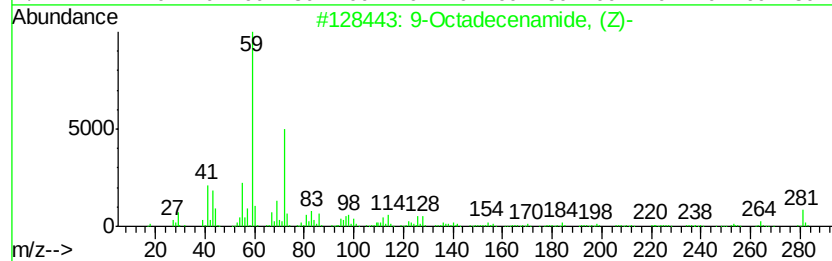
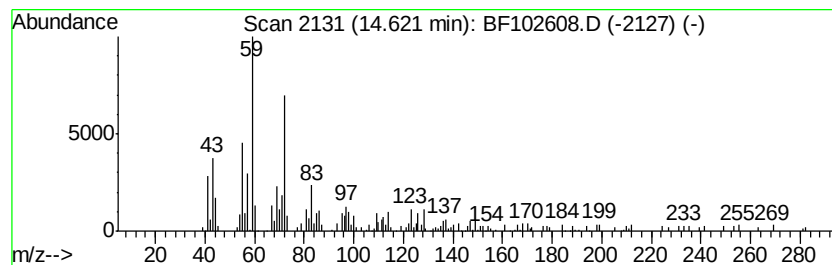
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Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	3.42 ng	182892	Perylene-d12	15.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
2		Dodecanamide	199	C12H25NO	001120-16-7	53
3		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	53
4		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	53
5		Acetic acid, cyanohydroxyimino-,...	128	C4H4N2O3	061295-92-9	43



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.93	2.7	ng	130091	1	6.71	959252	20.0
unknown6.49	6.49	85.9	ng	4122120	1	6.71	959252	20.0
Ethanol, 2-(2-eth...	6.55	3.1	ng	149216	1	6.71	959252	20.0
1-Docosene	13.71	10.4	ng	635057	5	13.88	1219310	20.0
9-Octadecenamide,...	14.62	3.4	ng	182892	6	15.31	1068660	20.0