

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030216\
 Data File : BF085121.D
 Acq On : 2 Mar 2016 16:05
 Operator : SJ/IZ
 Sample : H1620-02
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-02

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030116.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	2.573	20	25	29	rVB	283548	451648	8.40%	1.125%
2	2.710	35	37	48	rVB	91675	152230	2.83%	0.379%
3	4.276	171	174	177	rBV	75276	101234	1.88%	0.252%
4	5.201	252	255	258	rVB	262857	376555	7.00%	0.938%
5	5.602	287	290	292	rBV	3206060	3463588	64.38%	8.629%
6	6.607	376	378	381	rBV	1959290	2041236	37.94%	5.085%
7	6.756	388	391	394	rBV	3754739	4700216	87.37%	11.710%
8	6.996	409	412	414	rBV	982378	1012776	18.83%	2.523%
9	7.156	423	426	428	rVB	3130269	4031333	74.93%	10.043%
10	7.556	458	461	463	rBV	3319272	3276210	60.90%	8.162%
11	7.636	466	468	471	rVB2	61139	83667	1.56%	0.208%
12	8.276	522	524	526	rBV	1614050	1347841	25.05%	3.358%
13	8.608	551	553	556	rBV2	31245	59024	1.10%	0.147%
14	9.350	615	618	620	rBV	4744807	5379777	100.00%	13.403%
15	9.739	650	652	654	rVB	330347	290681	5.40%	0.724%
16	10.036	675	678	680	rBV	1413235	1428859	26.56%	3.560%
17	10.459	711	715	716	rVB3	45652	84307	1.57%	0.210%
18	10.825	744	747	749	rBV	3424806	3707047	68.91%	9.235%
19	10.928	754	756	761	rVB3	42402	74084	1.38%	0.185%
20	11.374	793	795	800	rBV2	28868	70298	1.31%	0.175%
21	11.522	805	808	810	rVB	1072076	1237816	23.01%	3.084%
22	11.739	825	827	830	rVB2	76327	93645	1.74%	0.233%
23	12.036	851	853	855	rBV	198446	193272	3.59%	0.482%
24	12.745	913	915	920	rBV3	47660	72982	1.36%	0.182%
25	12.825	920	922	924	rBV	120667	150259	2.79%	0.374%
26	13.099	944	946	949	rBV	3634031	3823500	71.07%	9.526%
27	13.568	985	987	989	rBV	46181	68087	1.27%	0.170%
28	13.625	990	992	994	rVV	78283	84873	1.58%	0.211%
29	13.945	1018	1020	1022	rBV	65691	85298	1.59%	0.213%
30	14.151	1036	1038	1041	rVB	976321	926441	17.22%	2.308%
31	14.665	1081	1083	1086	rBV	74032	146621	2.73%	0.365%
32	15.637	1165	1168	1171	rBV	855257	1123916	20.89%	2.800%

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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-BF030116.M
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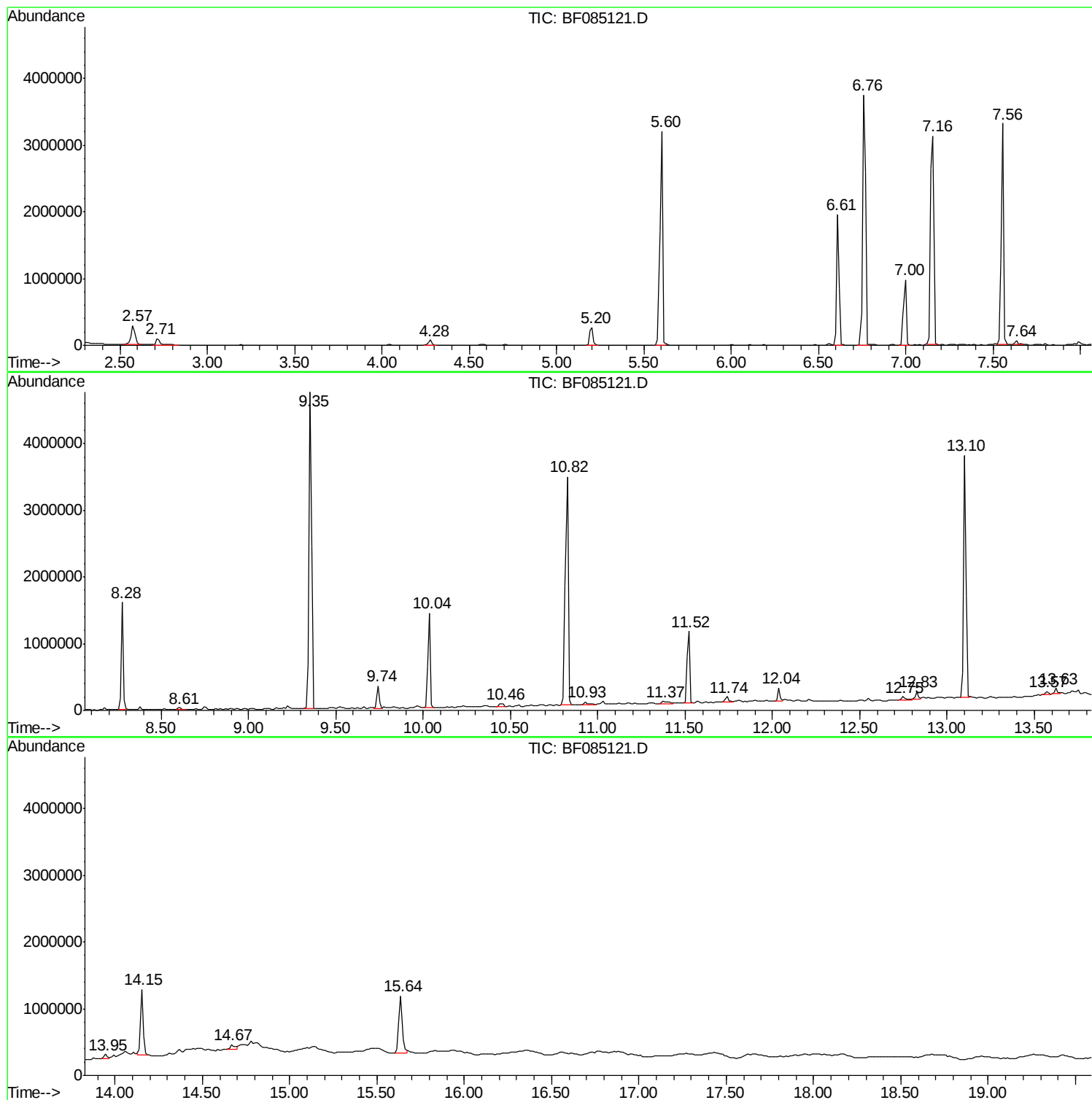
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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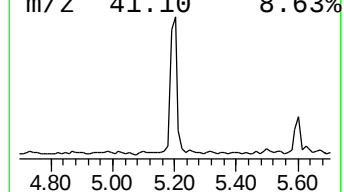
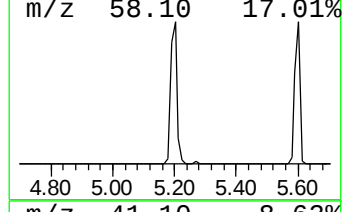
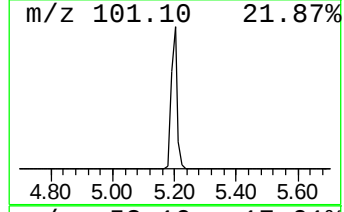
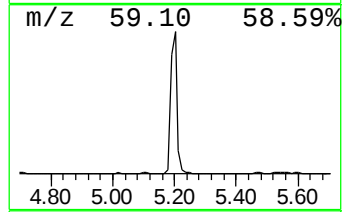
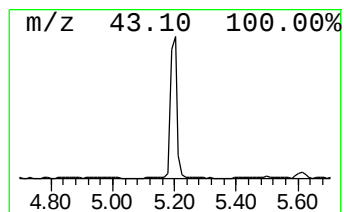
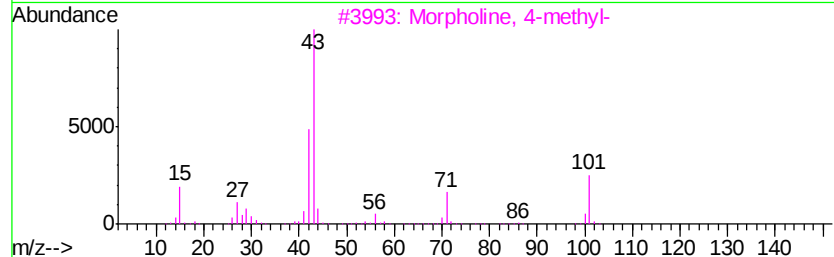
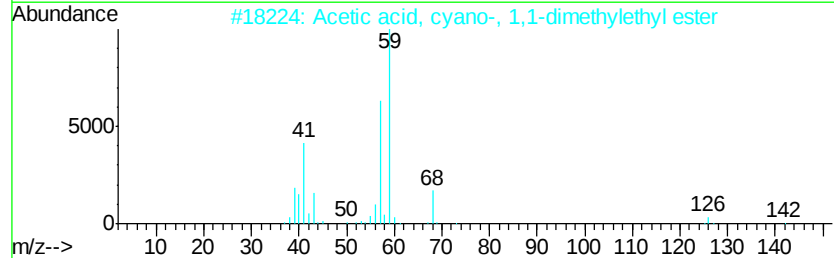
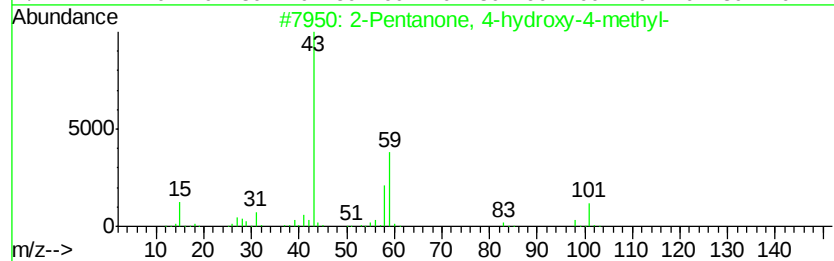
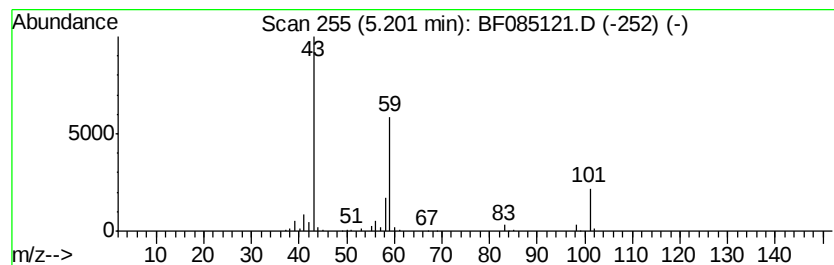
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	7.44 ng	376555	1,4-Dichlorobenzene-d4	7.00

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Butane	58	C4H10	000106-97-8	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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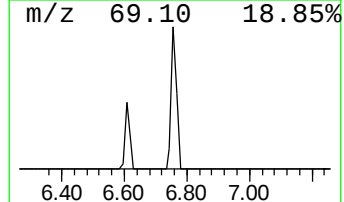
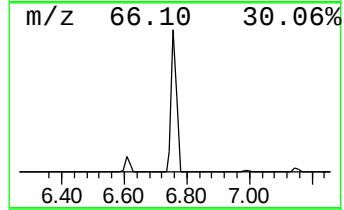
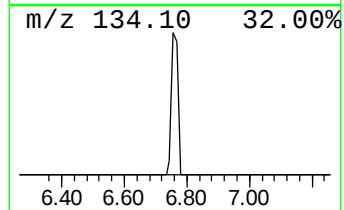
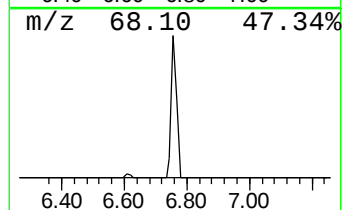
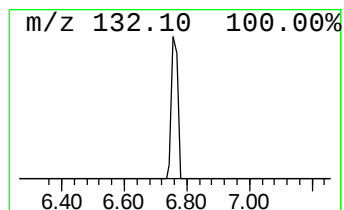
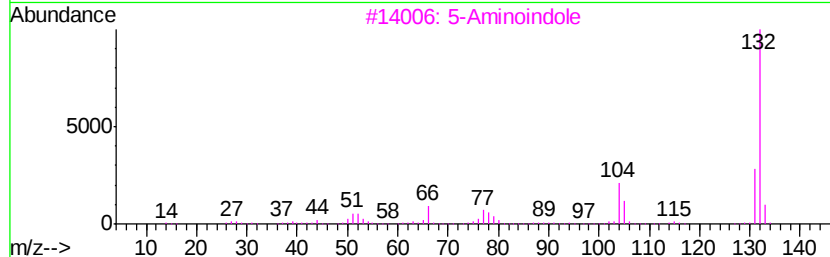
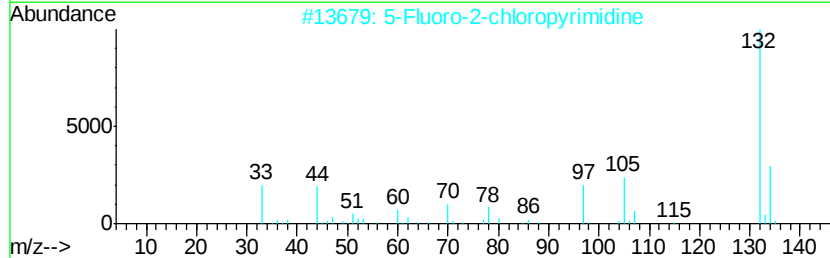
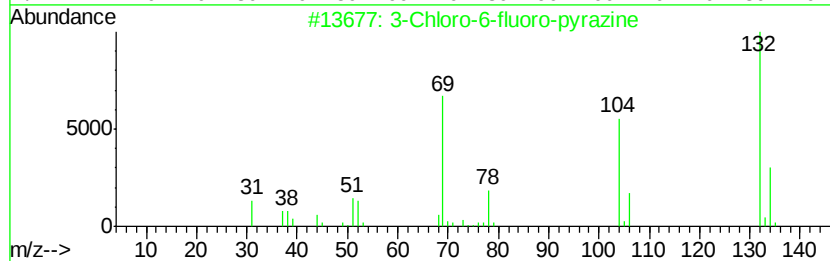
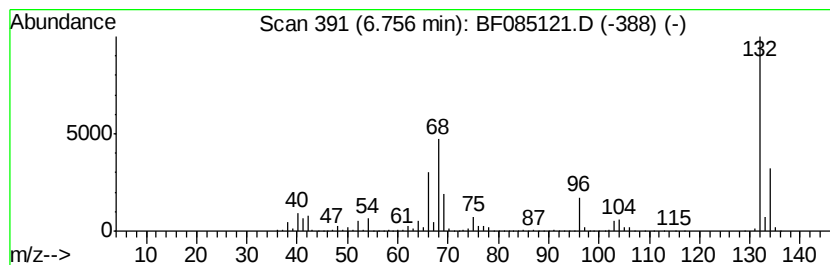
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.76 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.76	92.82 ng	4700220	1,4-Dichlorobenzene-d4	7.00

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		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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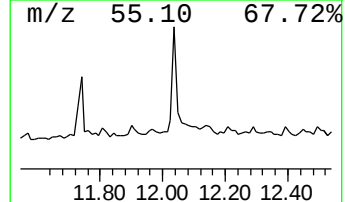
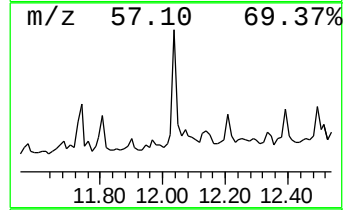
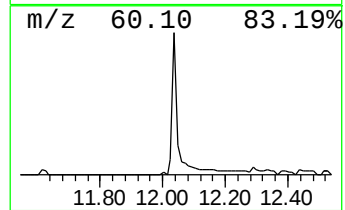
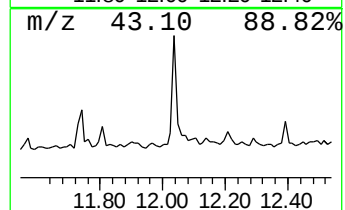
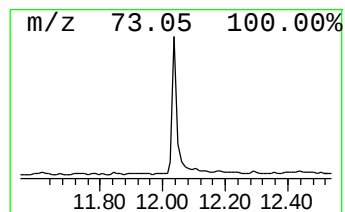
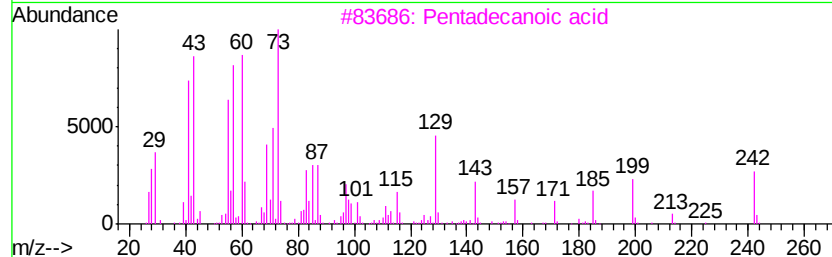
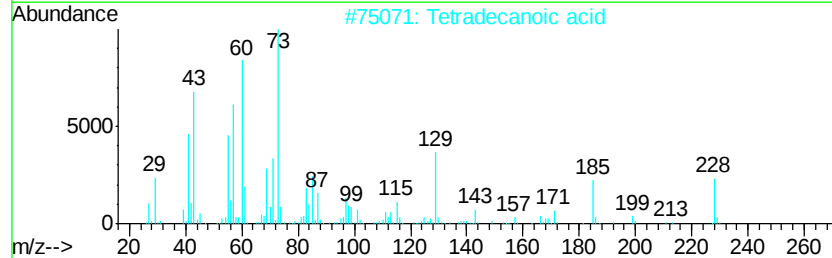
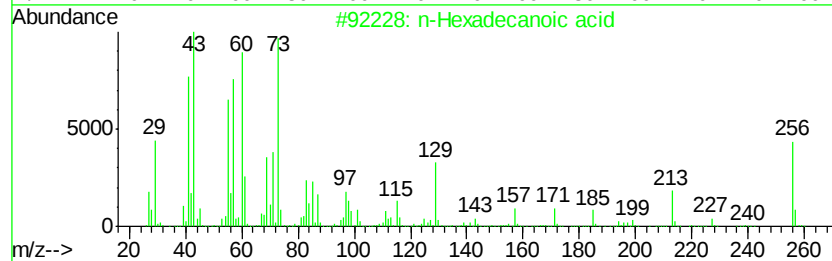
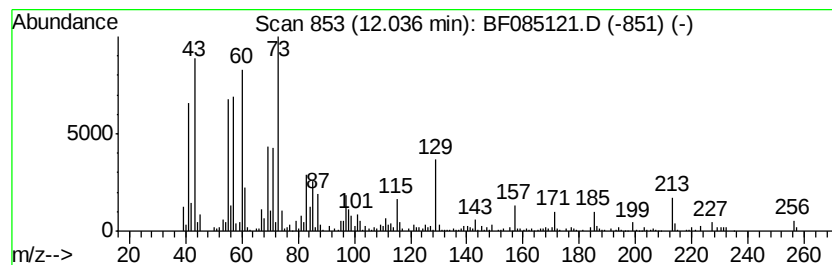
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.04	3.12 ng	193272	Phenanthrene-d10	11.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4		Tridecanoic acid	214	C13H26O2	000638-53-9	81
5		Tridecane	184	C13H28	000629-50-5	25



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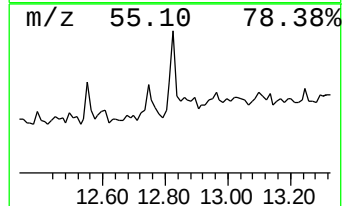
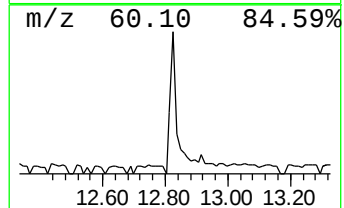
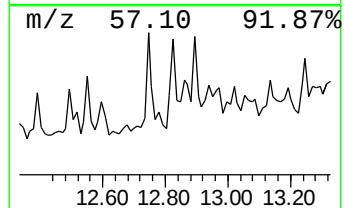
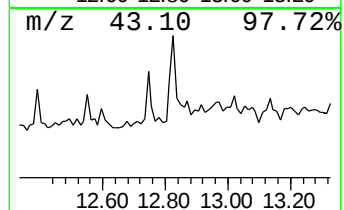
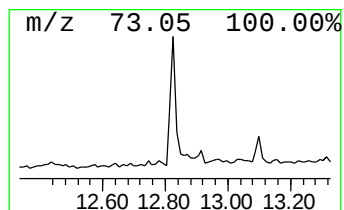
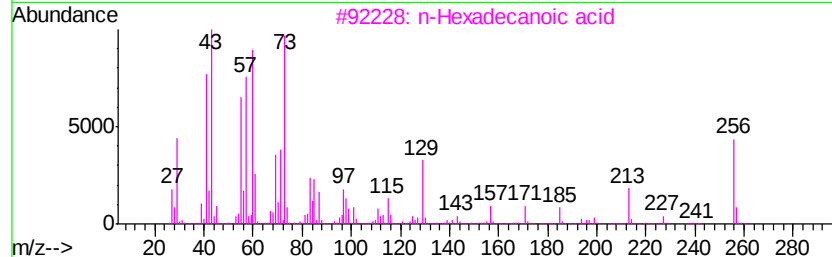
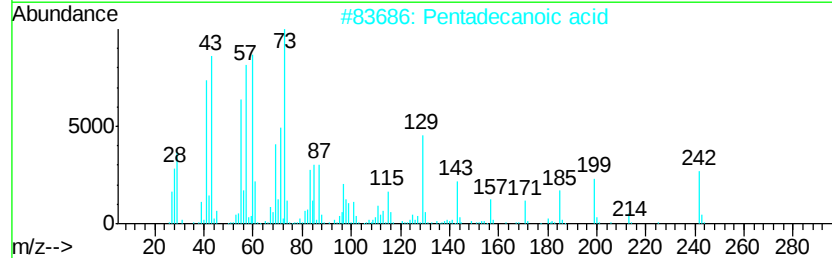
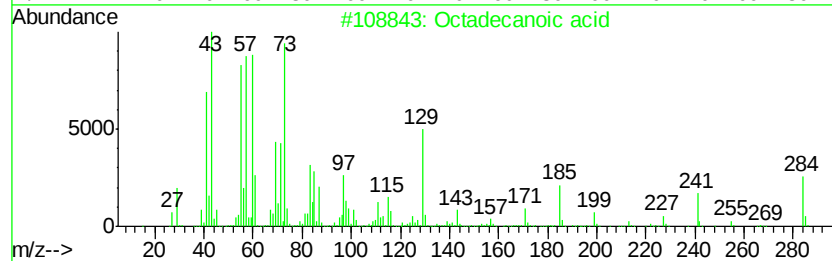
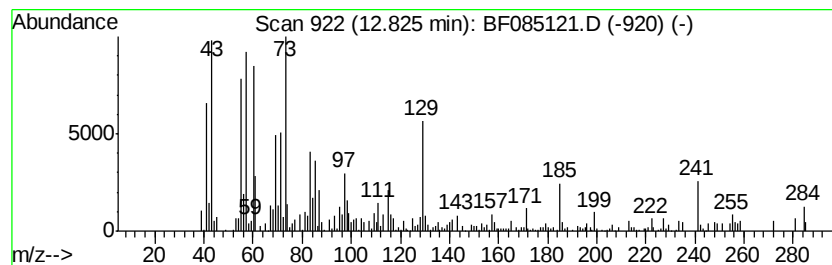
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.83	2.43 ng	150259	Phenanthrene-d10	11.52	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	59



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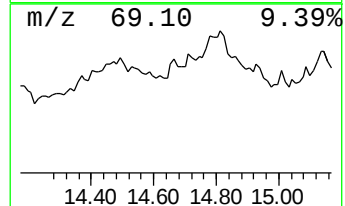
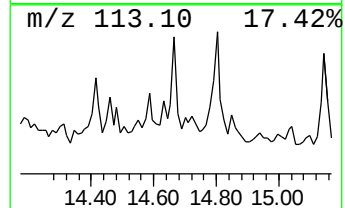
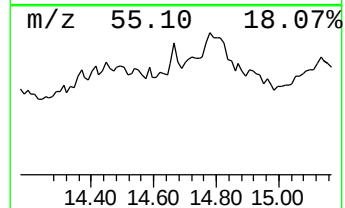
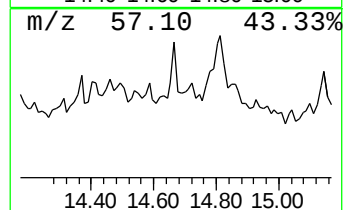
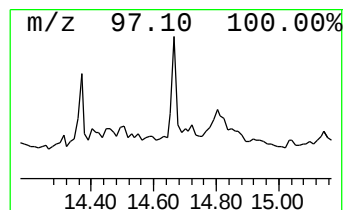
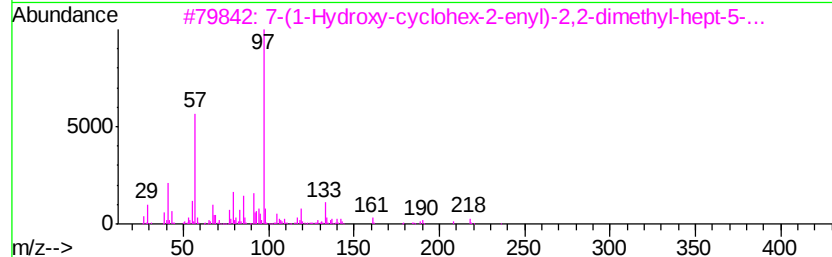
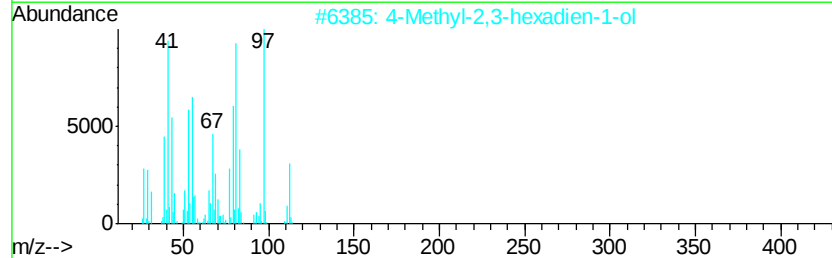
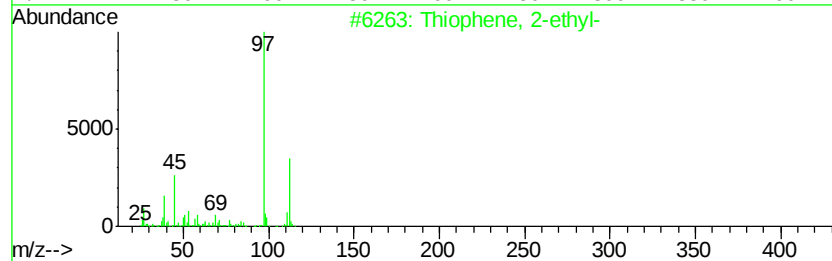
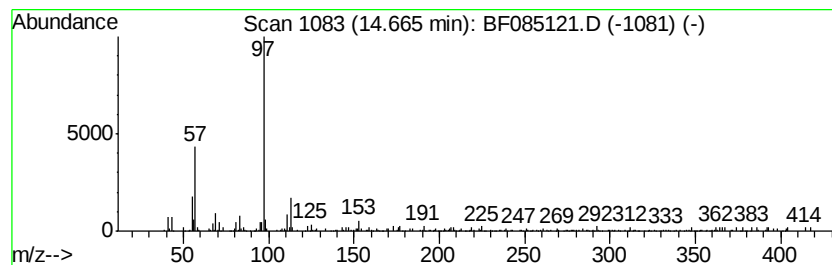
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Thiophene, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	3.17 ng	146621	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Thiophene, 2-ethyl-	112	C6H8S	000872-55-9	59
2		4-Methyl-2,3-hexadien-1-ol	112	C7H12O	1000196-09-6	58
3		7-(1-Hydroxy-cyclohex-2-enyl)-2,...	236	C15H24O2	083040-94-2	53
4		3-Cyclopent-1-enyl-3-hydroxy-2-m...	170	C9H14O3	1000191-19-7	53
5		Methylphosphonic acid, di(2-meth...	208	C9H21O3P	105263-11-4	42



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.20	7.4	ng	376555	1	7.00	1012780	20.0
unknown6.76	6.76	92.8	ng	4700220	1	7.00	1012780	20.0
n-Hexadecanoic acid	12.04	3.1	ng	193272	4	11.52	1237820	20.0
Octadecanoic acid	12.83	2.4	ng	150259	4	11.52	1237820	20.0
Thiophene, 2-ethyl-	14.67	3.2	ng	146621	5	14.15	926441	20.0