

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062516\
 Data File : BF088395.D
 Acq On : 26 Jun 2016 2:11
 Operator : UM/SJ
 Sample : H3745-04
 Misc :
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-08-COMP

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-BF060716.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	1.678	6	8	9	rBV	22012	26928	1.61%	0.195%
2	1.701	9	10	38	rVB	354126	675428	40.48%	4.896%
3	4.684	268	271	284	rBV	71131	124824	7.48%	0.905%
4	5.141	309	311	335	rBV	1026404	1373236	82.30%	9.953%
5	6.227	403	406	413	rBV	1211460	1380014	82.71%	10.003%
6	6.330	413	415	433	rVB	1457979	1483756	88.92%	10.754%
7	6.559	433	435	446	rBV	312866	348460	20.88%	2.526%
8	6.719	446	449	451	rBV	818166	1122168	67.25%	8.134%
9	7.130	483	485	488	rBV	553443	798657	47.86%	5.789%
10	7.850	546	548	550	rBV	353419	448745	26.89%	3.253%
11	8.925	639	642	644	rBV	1766409	1668573	100.00%	12.094%
12	9.325	675	677	686	rVB	115888	100993	6.05%	0.732%
13	9.588	698	700	703	rBV	563243	526678	31.56%	3.817%
14	10.376	767	769	779	rBV	739242	810515	48.58%	5.875%
15	10.502	779	780	787	rVB	18199	26936	1.61%	0.195%
16	10.948	817	819	821	rBV	38015	37026	2.22%	0.268%
17	11.062	827	829	833	rBV	411150	438836	26.30%	3.181%
18	11.131	833	835	839	rVB	14162	26695	1.60%	0.193%
19	11.325	849	852	855	rBV	11458	22312	1.34%	0.162%
20	11.371	855	856	859	rVB	21540	20287	1.22%	0.147%
21	12.479	951	953	956	rBV	51998	49170	2.95%	0.356%
22	12.651	965	968	970	rBV	1004265	1236063	74.08%	8.959%
23	13.188	1012	1015	1016	rBV	22537	29095	1.74%	0.211%
24	13.554	1045	1047	1056	rBV	35974	84396	5.06%	0.612%
25	13.691	1056	1059	1066	rVV	372255	399815	23.96%	2.898%
26	14.194	1099	1103	1110	rBV2	11794	39844	2.39%	0.289%
27	14.445	1123	1125	1128	rBV2	10429	21531	1.29%	0.156%
28	14.754	1150	1152	1153	rBV	16796	18709	1.12%	0.136%
29	15.040	1175	1177	1183	rBV	211424	318990	19.12%	2.312%
30	15.417	1207	1210	1214	rBV	23962	32212	1.93%	0.233%
31	15.508	1214	1218	1223	rVV6	5679	18879	1.13%	0.137%
32	15.817	1243	1245	1250	rVB2	11882	24292	1.46%	0.176%
33	16.297	1283	1287	1289	rBV	11010	24506	1.47%	0.178%
34	16.468	1299	1302	1306	rVB4	9085	18523	1.11%	0.134%

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ALS Vial : 43 Sample Multiplier: 1

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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

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35	17.508	1387	1393	1398	rVB5	5844	19552	1.17%	0.142%
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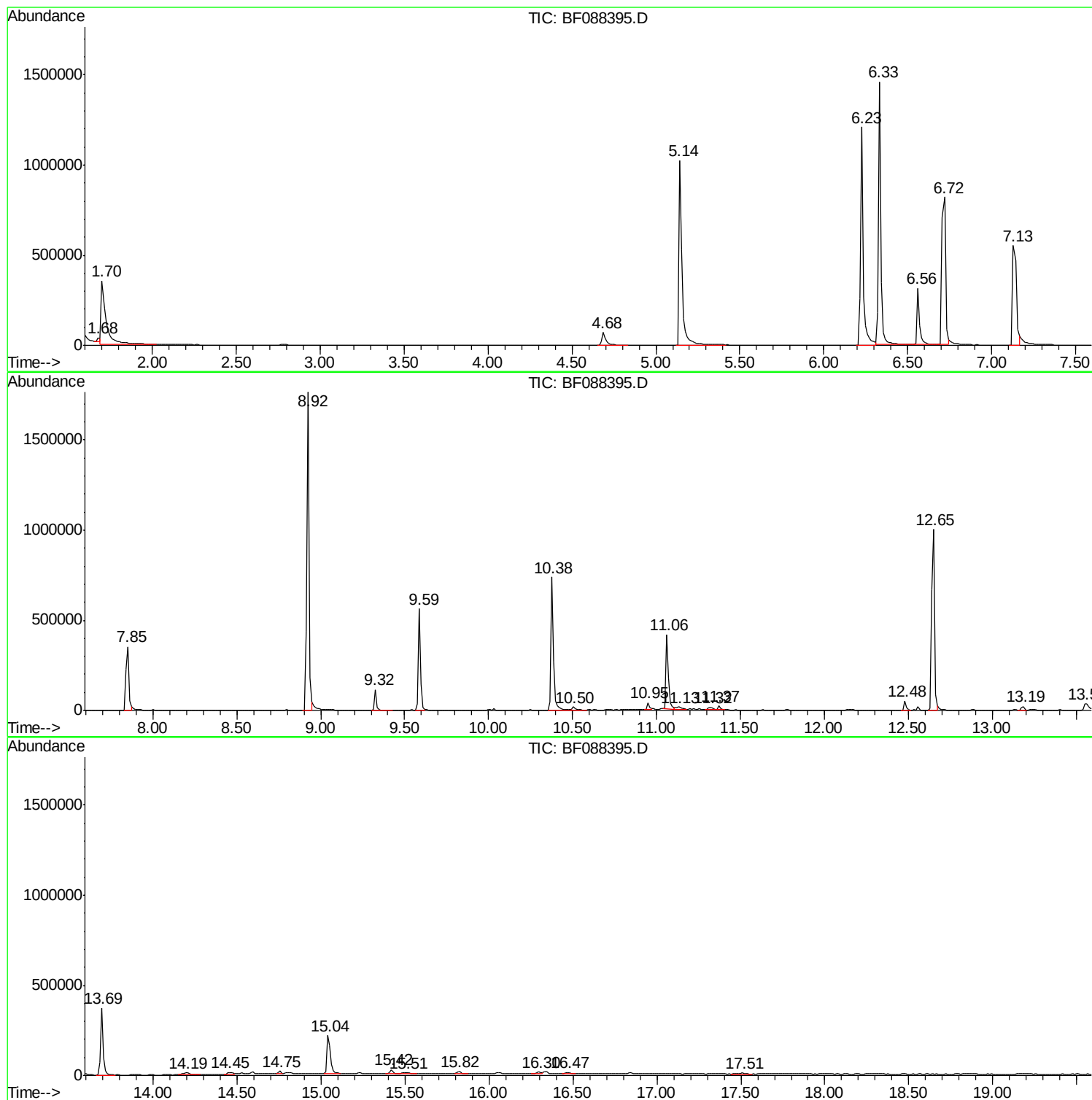
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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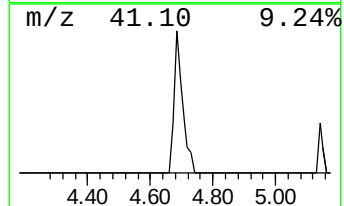
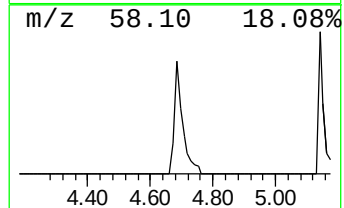
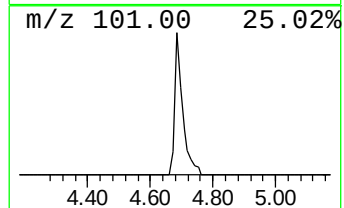
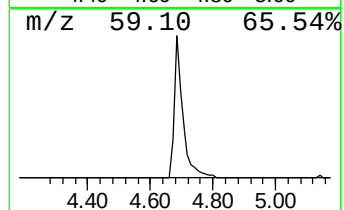
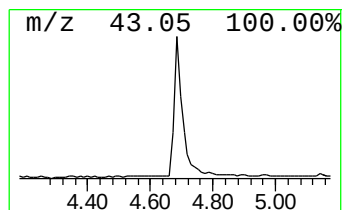
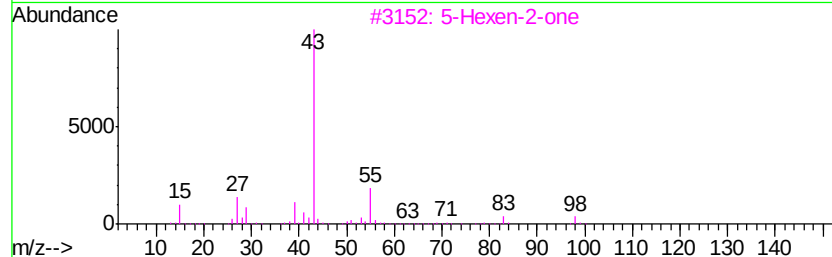
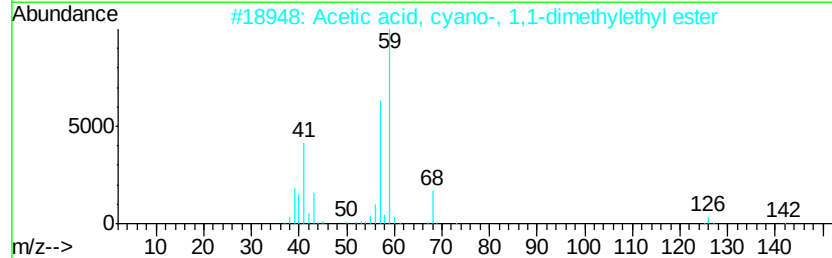
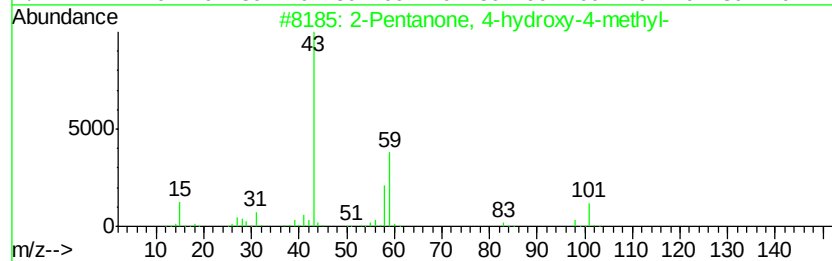
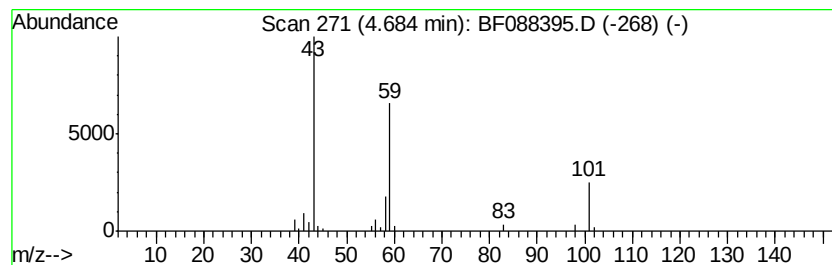
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TIC Library : C:\Database\NIST11.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.68	7.16 ng	124824	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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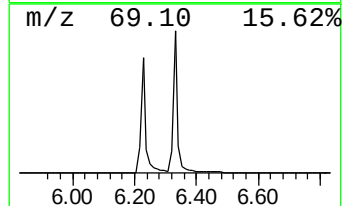
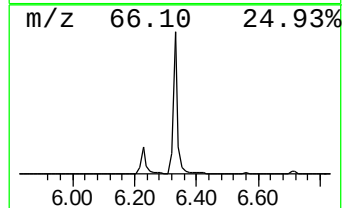
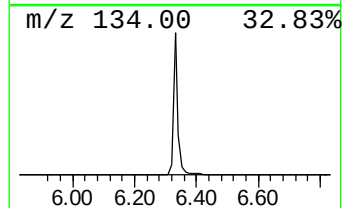
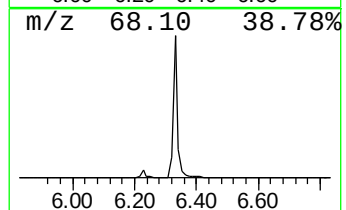
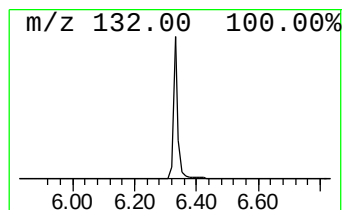
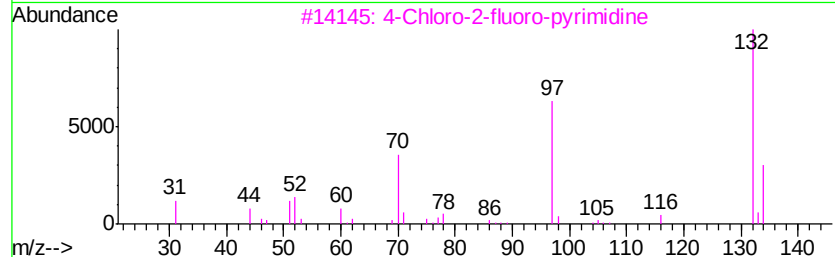
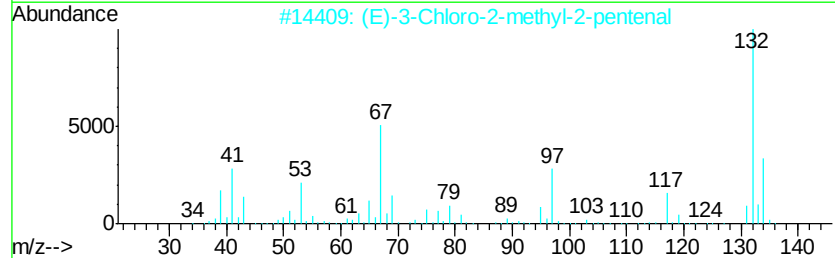
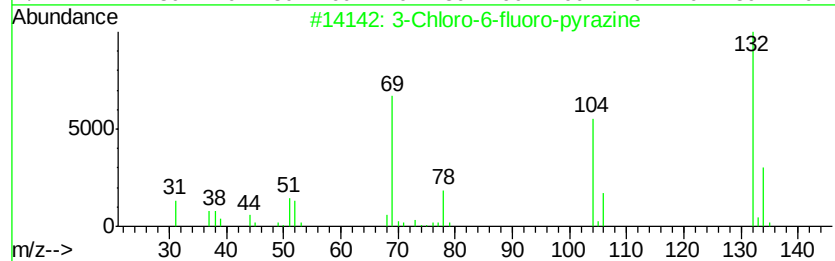
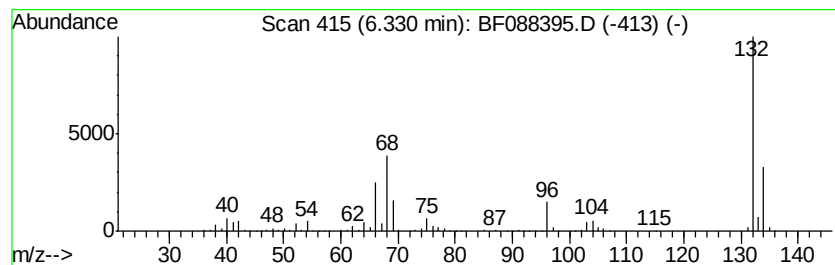
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TIC Library : C:\Database\NIST11.L
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Peak Number 3 unknown6.33 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.33	85.16 ng	1483760	1,4-Dichlorobenzene-d4	6.56

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		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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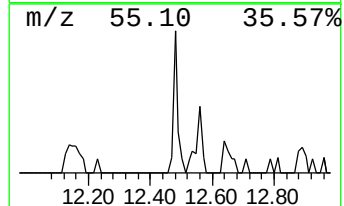
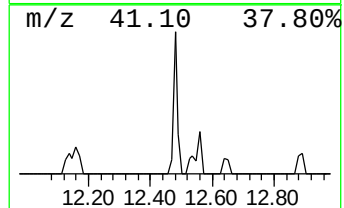
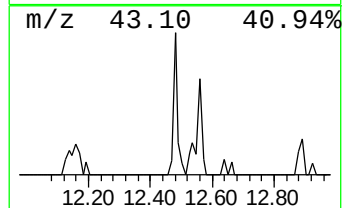
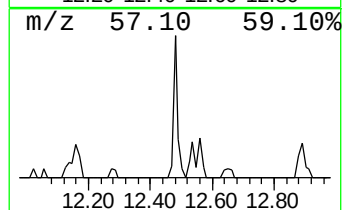
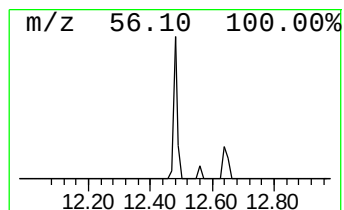
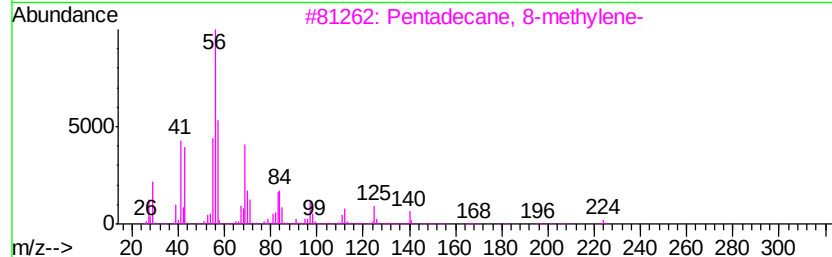
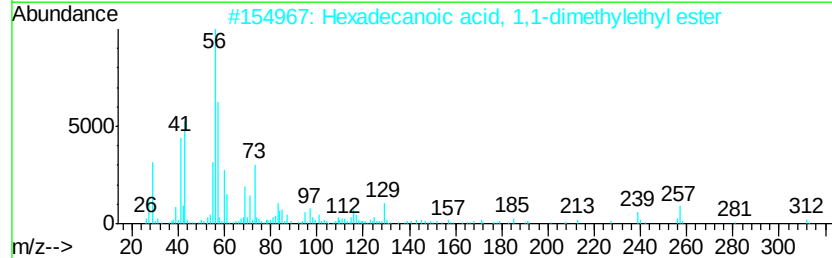
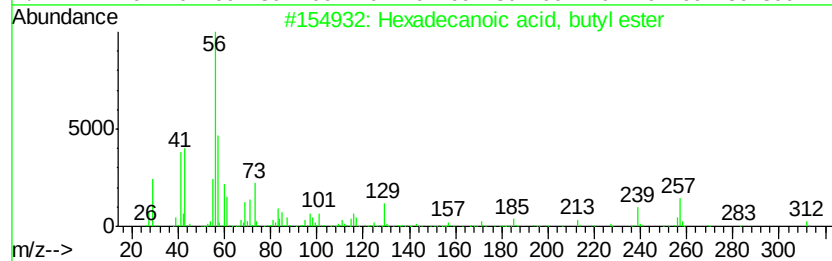
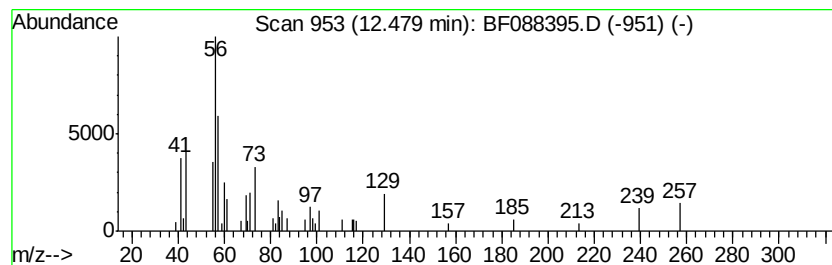
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	2.46 ng	49170	Chrysene-d12	13.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	83
3		Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32
4		2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	27
5		Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	25



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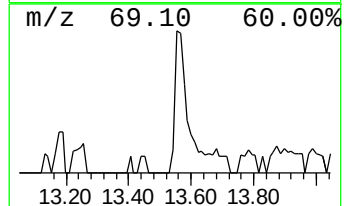
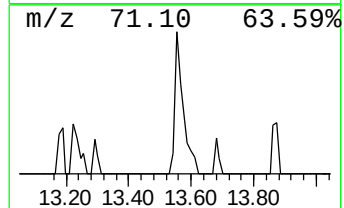
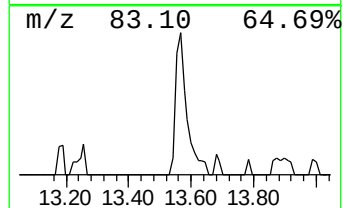
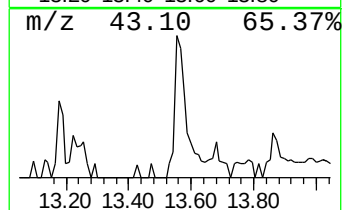
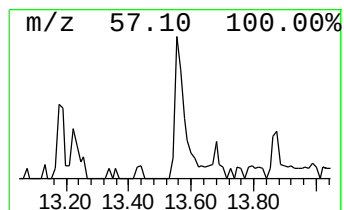
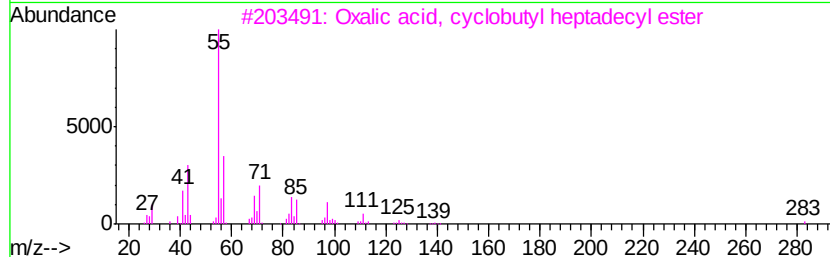
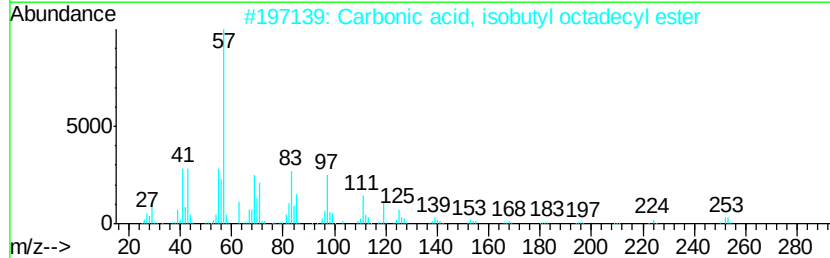
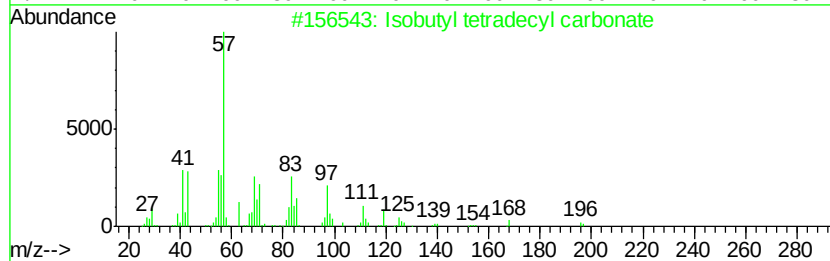
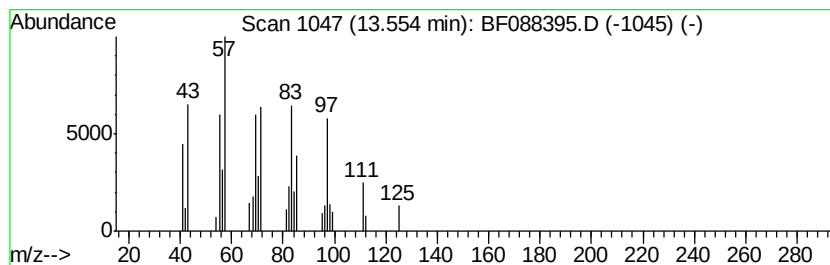
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 Isobutyl tetradecyl carbonate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	4.22 ng	84396	Chrysene-d12	13.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	91
2		Carbonic acid, isobutyl octadecyl...	370	C23H46O3	1000314-61-5	86
3		Oxalic acid, cyclobutyl heptadecyl...	382	C23H42O4	1000309-70-7	80
4		Oxalic acid, cyclobutyl octadecyl...	396	C24H44O4	1000309-70-8	72
5		2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	72



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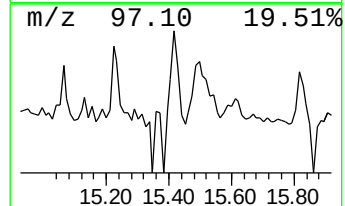
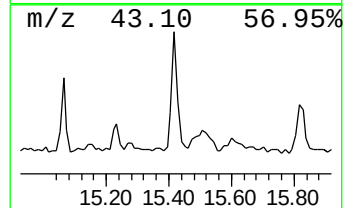
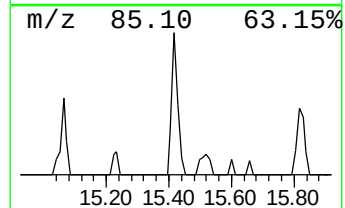
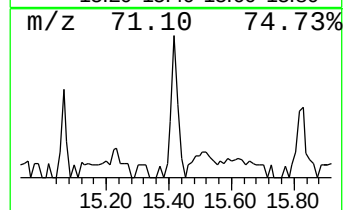
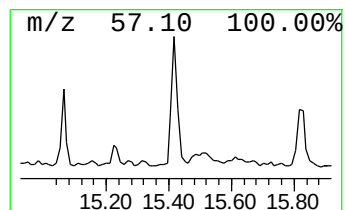
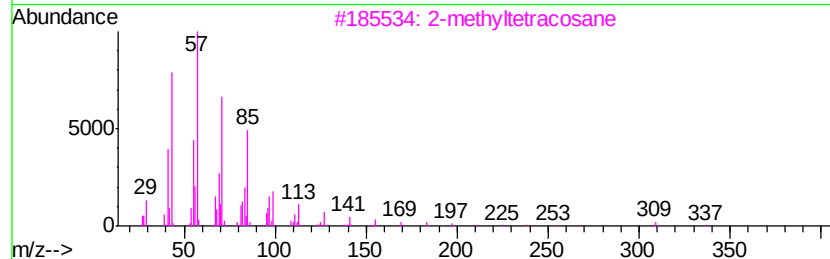
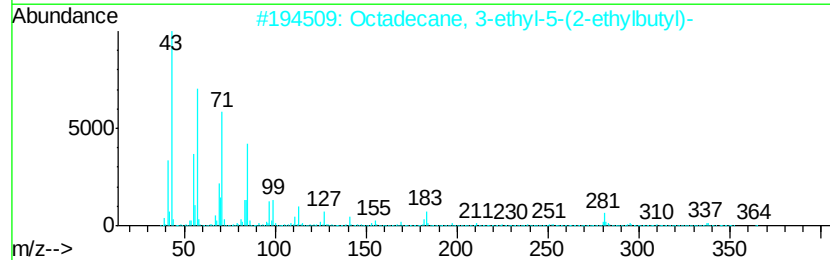
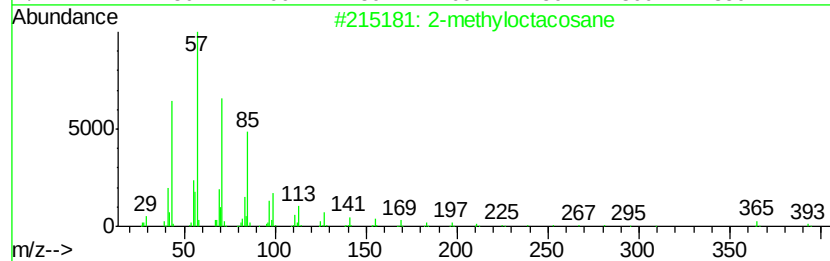
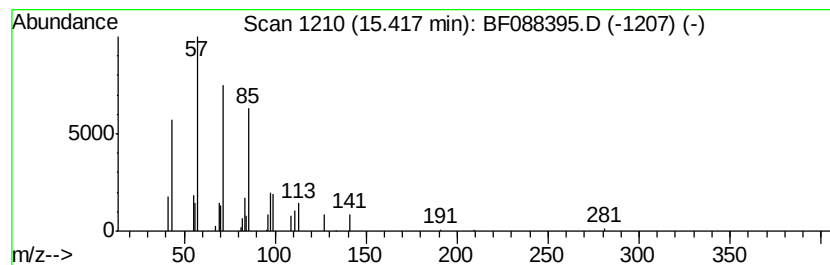
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Peak Number 7 2-methyloctacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.42	2.02 ng	32212	Perylene-d12	15.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	90
2		Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	90
3		2-methyltetracosane	352	C25H52	1000376-72-6	90
4		Heneicosane	296	C21H44	000629-94-7	86
5		Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	83



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.68	7.2	ng	124824	1	6.56	348460	20.0
unknown6.33	6.33	85.2	ng	1483760	1	6.56	348460	20.0
Hexadecanoic acid...	12.48	2.5	ng	49170	5	13.69	399815	20.0
Isobutyl tetradec...	13.55	4.2	ng	84396	5	13.69	399815	20.0
2-methyloctacosane	15.42	2.0	ng	32212	6	15.04	318990	20.0