

Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
 Data File : BF102744.D
 Acq On : 5 Feb 2018 18:06
 Operator : SJ/JU
 Sample : J1453-05
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P-2

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-BF020318.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	2.199	9	19	26	rVB	640197	857042	14.74%	1.746%
2	5.128	514	517	526	rVB	156407	212507	3.65%	0.433%
3	5.504	575	581	584	rBV	5367927	5815256	100.00%	11.848%
4	6.510	745	752	759	rBV	4906206	5764838	99.13%	11.745%
5	6.651	771	776	779	rBV	5283030	5658999	97.31%	11.530%
6	6.881	811	815	818	rBV	1618956	1265750	21.77%	2.579%
7	7.039	837	842	845	rVB	4633575	4309312	74.10%	8.780%
8	7.445	905	911	914	rBV	3595826	3714443	63.87%	7.568%
9	8.163	1029	1033	1036	rBV	2049305	1701073	29.25%	3.466%
10	9.239	1210	1216	1219	rBV	5803009	5609819	96.47%	11.429%
11	9.627	1278	1282	1285	rBV	895419	670487	11.53%	1.366%
12	9.816	1310	1314	1323	rVB	82760	142707	2.45%	0.291%
13	9.916	1327	1331	1335	rBV	1863866	1753043	30.15%	3.572%
14	10.633	1449	1453	1456	rBV	151824	139652	2.40%	0.285%
15	10.710	1460	1466	1469	rBV	3107604	3097558	53.27%	6.311%
16	11.404	1580	1584	1587	rBV	1737154	1457919	25.07%	2.970%
17	11.921	1669	1672	1680	rBV	358958	404645	6.96%	0.824%
18	12.615	1787	1790	1795	rBV	59488	80289	1.38%	0.164%
19	12.710	1802	1806	1815	rBV	114840	143500	2.47%	0.292%
20	12.880	1832	1835	1841	rVB	115319	96090	1.65%	0.196%
21	12.992	1849	1854	1857	rBV	4028432	3778234	64.97%	7.698%
22	13.463	1929	1934	1938	rVB3	52753	77832	1.34%	0.159%
23	13.874	2001	2004	2011	rBV	206813	202173	3.48%	0.412%
24	14.039	2028	2032	2036	rBV	1170149	1051397	18.08%	2.142%
25	15.521	2278	2284	2294	rVB	735007	988018	16.99%	2.013%
26	17.598	2634	2637	2644	rVB8	46919	90012	1.55%	0.183%

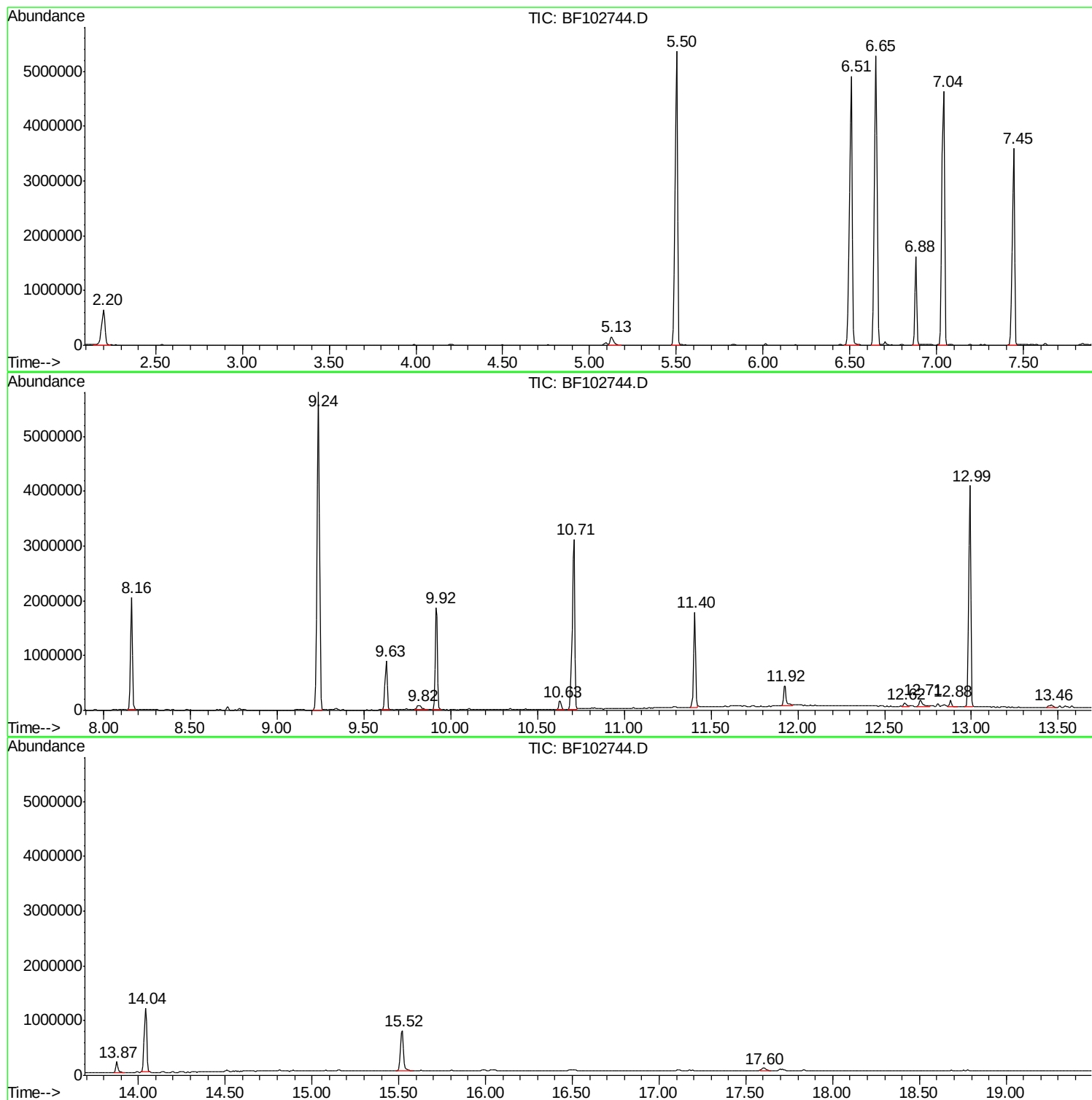
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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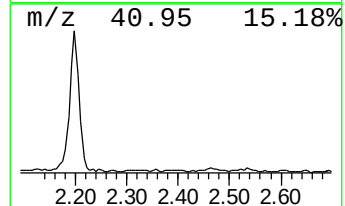
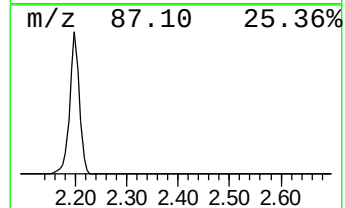
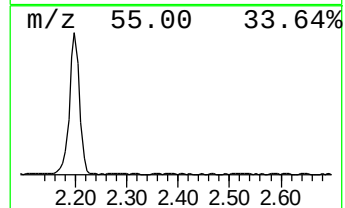
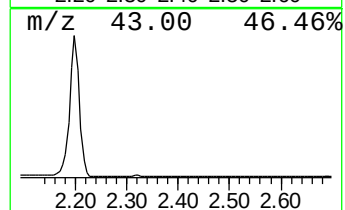
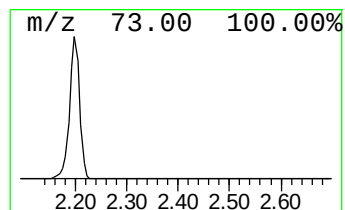
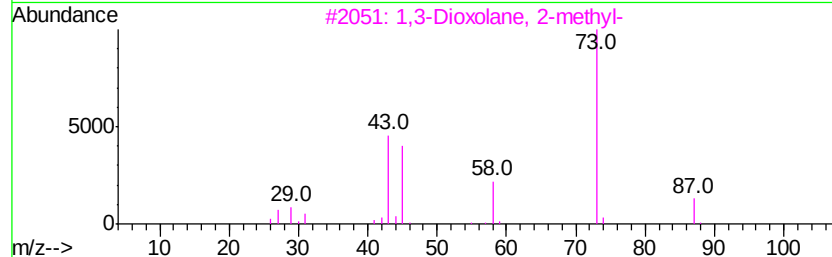
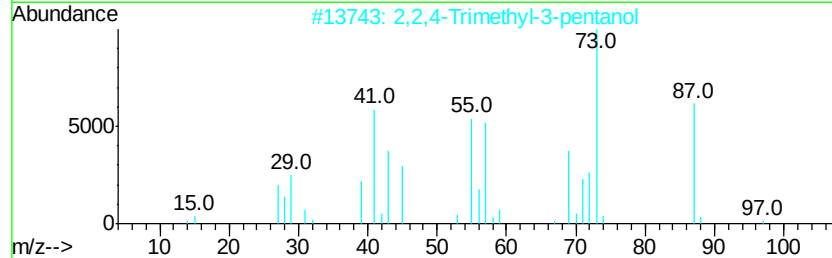
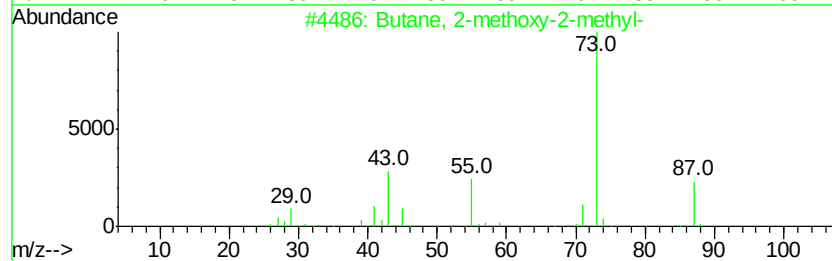
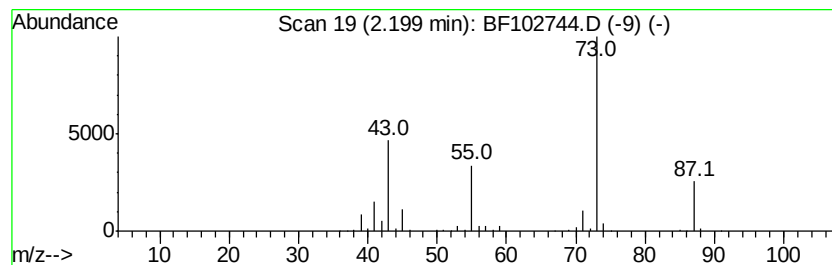
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	13.54 ng	857042	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
4		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
5		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23



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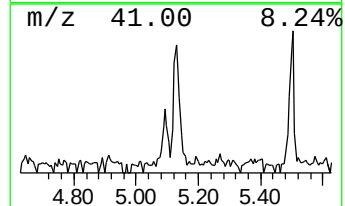
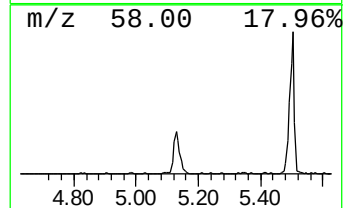
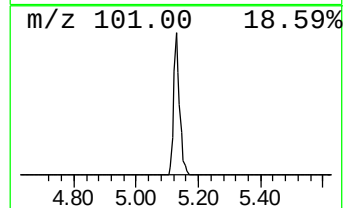
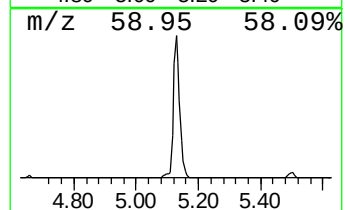
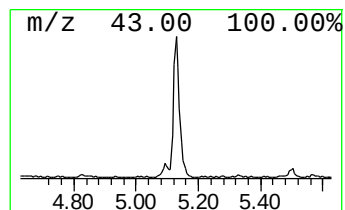
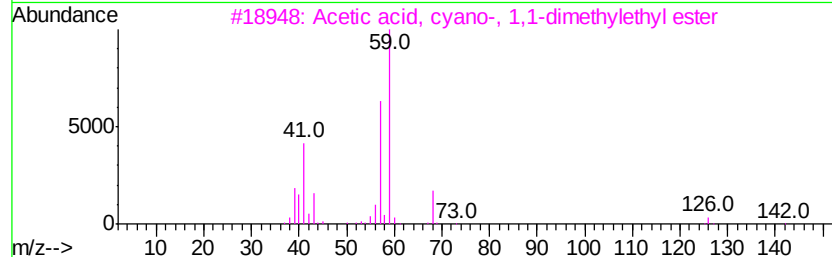
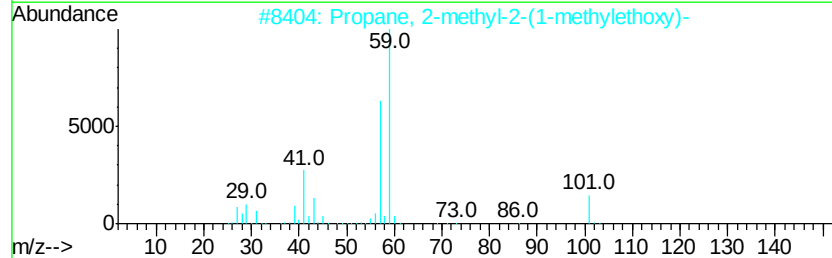
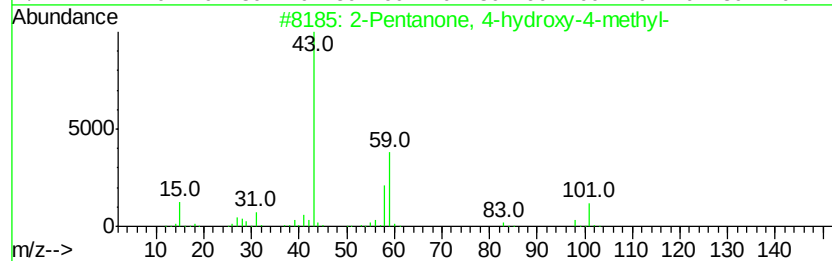
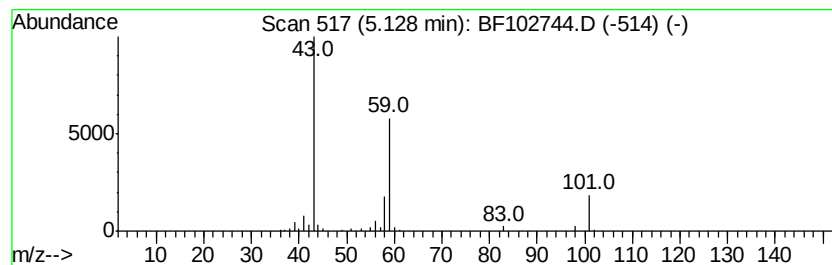
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	3.36 ng	212507	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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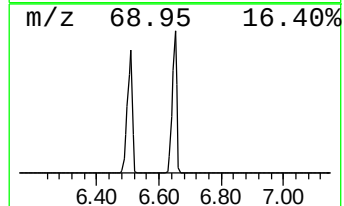
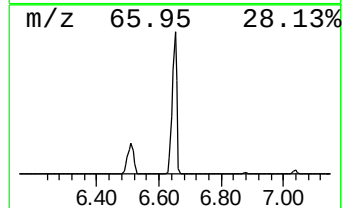
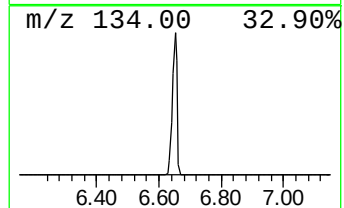
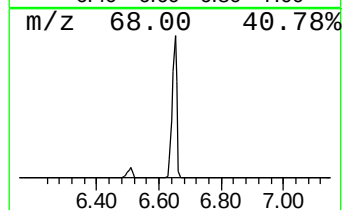
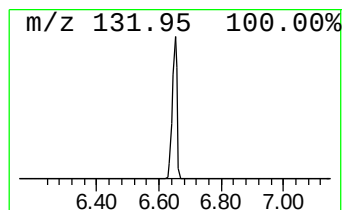
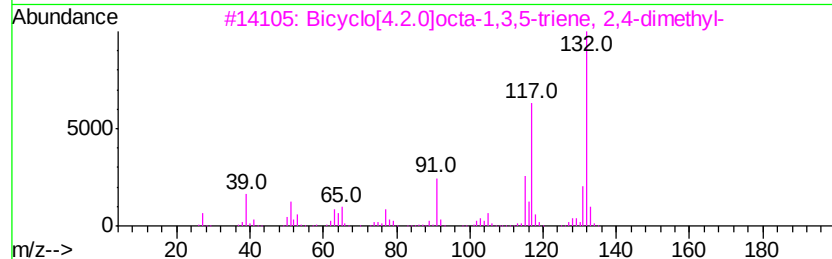
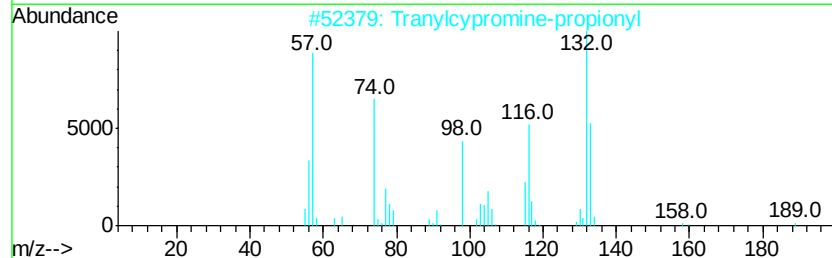
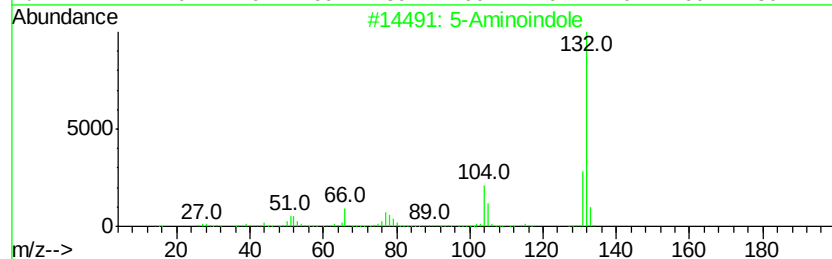
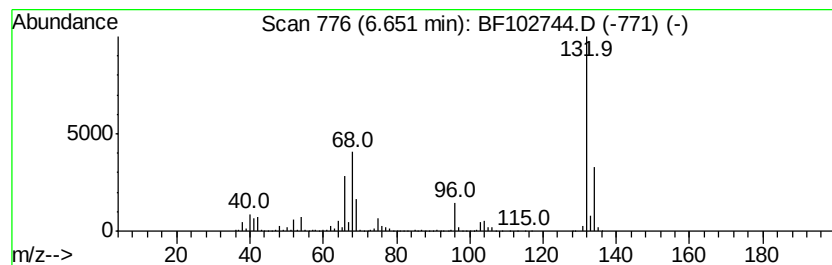
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Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	89.42 ng	5659000	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	12
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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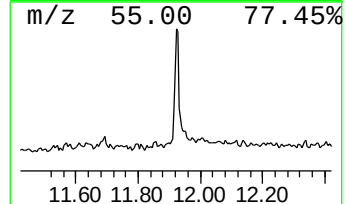
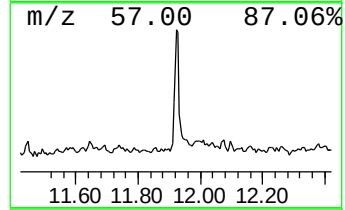
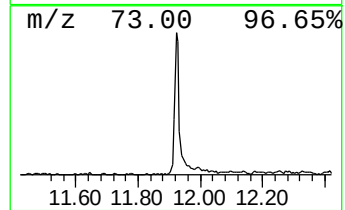
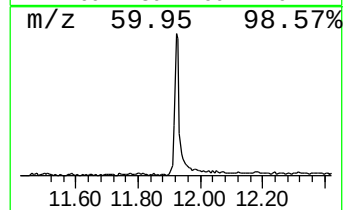
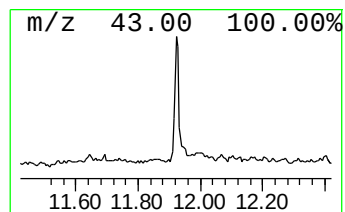
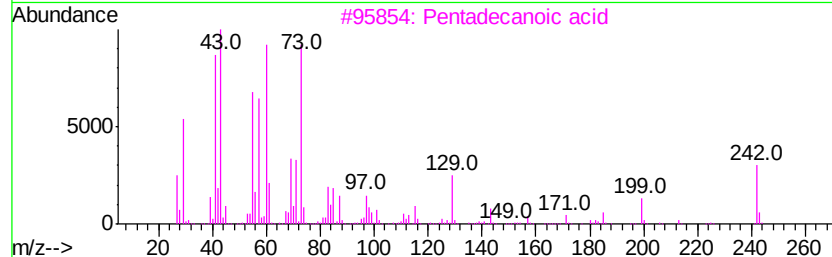
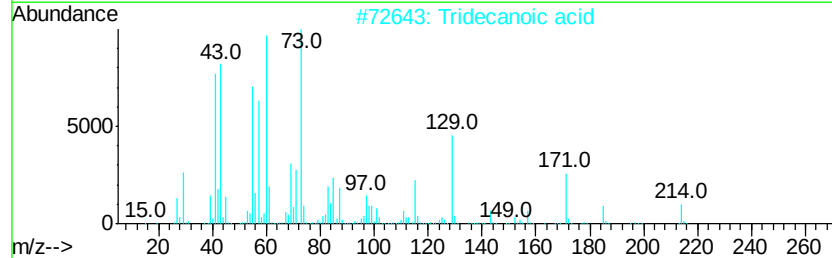
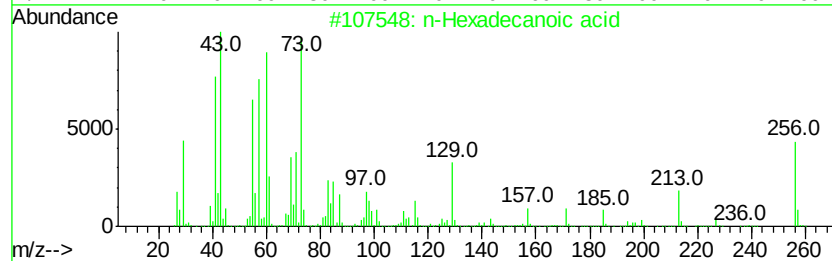
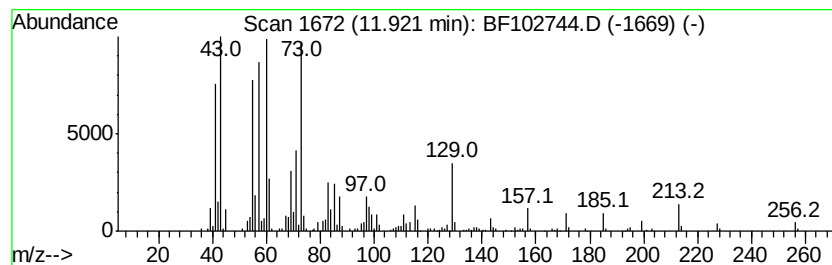
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	5.55 ng	404645	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	Undecanoic acid	186	C11H22O2	000112-37-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70



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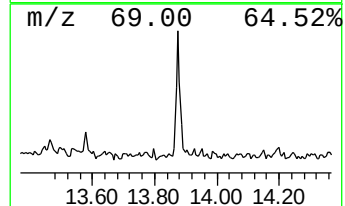
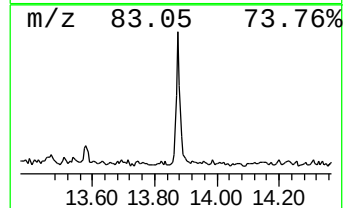
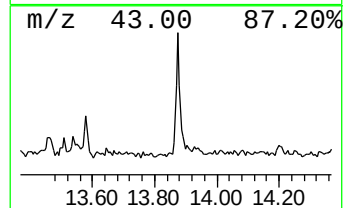
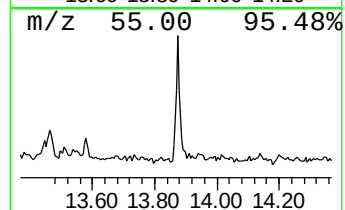
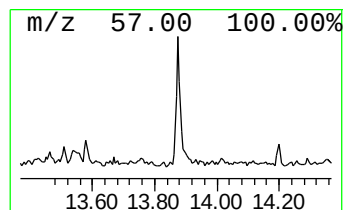
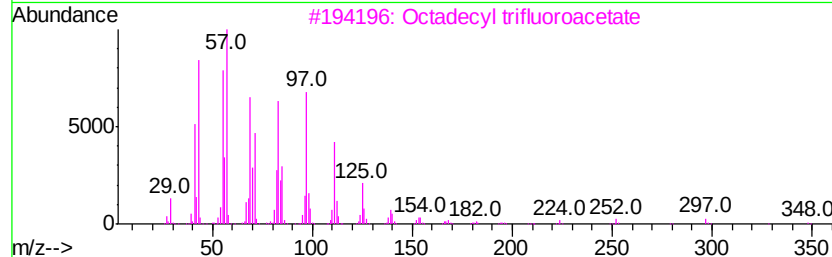
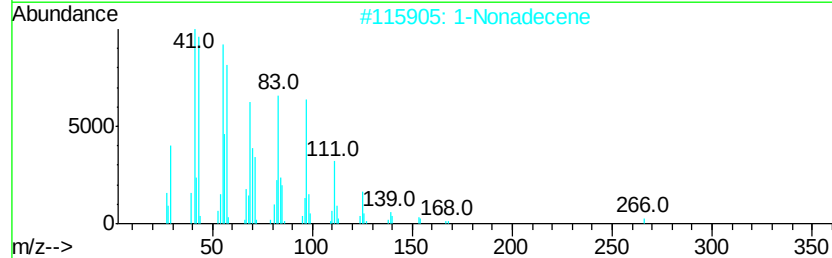
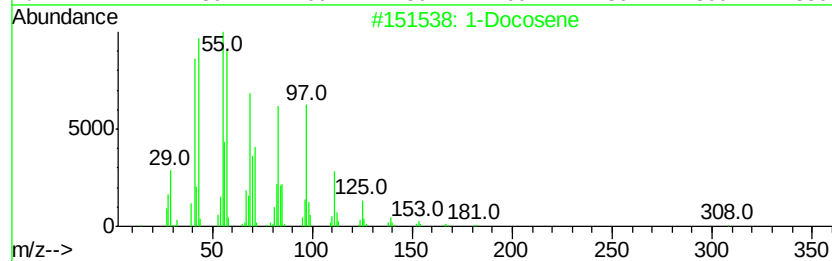
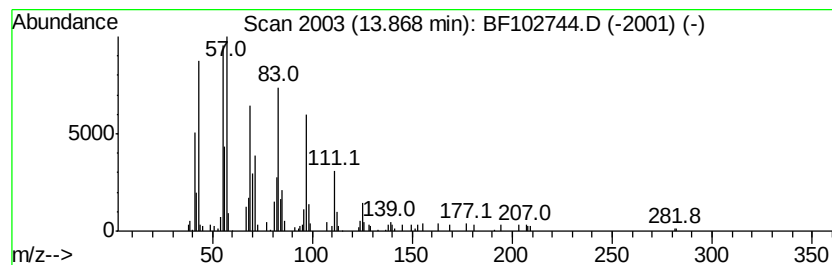
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.87	3.85 ng	202173	Chrysene-d12	14.04	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	94
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.20	13.5	ng	857042	1	6.88	1265750	20.0
2-Pentanone, 4-hy...	5.13	3.4	ng	212507	1	6.88	1265750	20.0
unknown6.65	6.65	89.4	ng	5659000	1	6.88	1265750	20.0
n-Hexadecanoic acid	11.92	5.5	ng	404645	4	11.40	1457920	20.0
1-Docosene	13.87	3.9	ng	202173	5	14.04	1051400	20.0