

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052121\
 Data File : BF124029.D
 Acq On : 21 May 2021 21:04
 Operator : JU/CG
 Sample : M2479-03
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GROUND-MATERIAL-1-17-D

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124029.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	8	16	22	rVB	577360	736400	50.53%	6.359%
2	2.287	29	34	39	rBV	49606	59517	4.08%	0.514%
3	5.110	509	514	521	rVB	184447	227830	15.63%	1.967%
4	5.510	577	582	585	rBV	1416195	1293250	88.75%	11.167%
5	5.904	646	649	652	rBB	23052	18609	1.28%	0.161%
6	6.516	747	753	756	rBV	1341819	1334581	91.58%	11.524%
7	6.710	784	786	793	rBV	38351	31741	2.18%	0.274%
8	6.886	813	816	820	rBV	450949	396512	27.21%	3.424%
9	7.451	907	912	915	rBV	1085807	898982	61.69%	7.763%
10	8.175	1031	1035	1038	rVB	643650	518841	35.60%	4.480%
11	9.245	1213	1217	1221	rBV	1622936	1457264	100.00%	12.583%
12	9.363	1233	1237	1240	rVB	30156	28415	1.95%	0.245%
13	9.639	1280	1284	1288	rBV	239751	182357	12.51%	1.575%
14	9.927	1329	1333	1336	rBV	779053	606201	41.60%	5.234%
15	10.716	1463	1467	1470	rBV	1156218	952444	65.36%	8.224%
16	11.416	1582	1586	1589	rBV	682171	541646	37.17%	4.677%
17	11.939	1670	1675	1677	rBV2	26152	24470	1.68%	0.211%
18	13.004	1851	1856	1859	rBV	1290372	1144303	78.52%	9.881%
19	13.898	2004	2008	2019	rBV2	147427	210836	14.47%	1.821%
20	14.057	2031	2035	2038	rVB	488332	415271	28.50%	3.586%
21	14.539	2113	2117	2120	rBV6	15166	19162	1.31%	0.165%
22	14.921	2179	2182	2185	rVB5	16377	18015	1.24%	0.156%
23	15.180	2224	2226	2231	rVB6	12290	20326	1.39%	0.176%
24	15.545	2283	2288	2293	rBV2	280549	354749	24.34%	3.063%
25	16.033	2367	2371	2375	rBV6	18511	26941	1.85%	0.233%
26	16.098	2377	2382	2385	rBV6	22170	37784	2.59%	0.326%
27	17.850	2674	2680	2683	rBV6	13536	24462	1.68%	0.211%

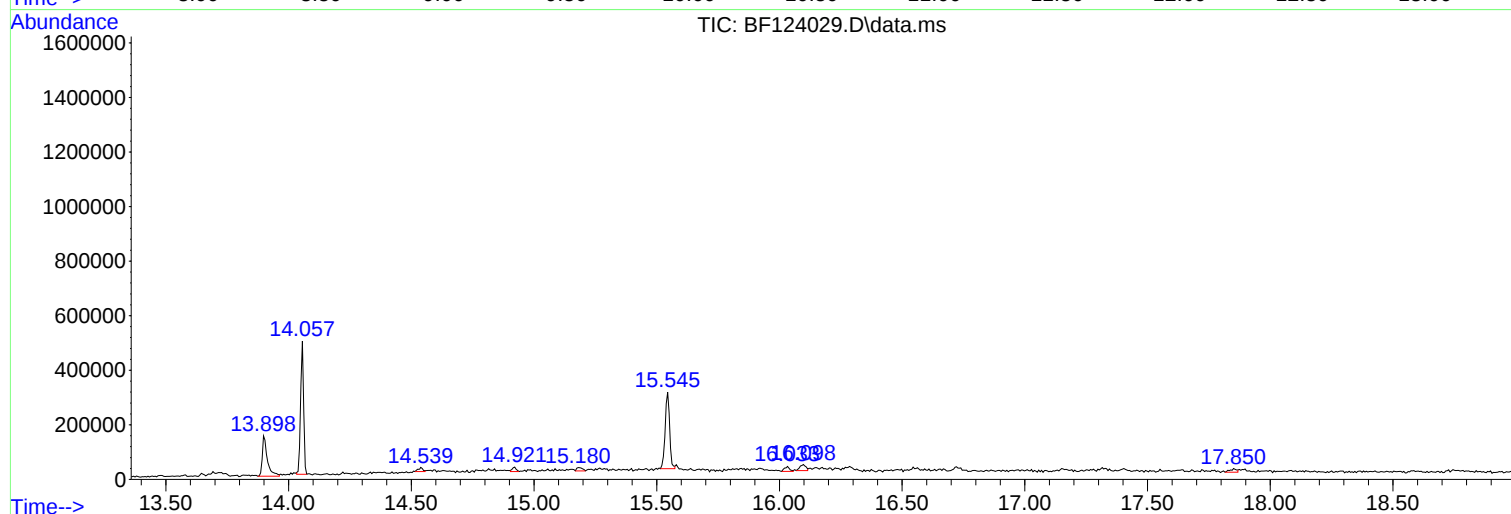
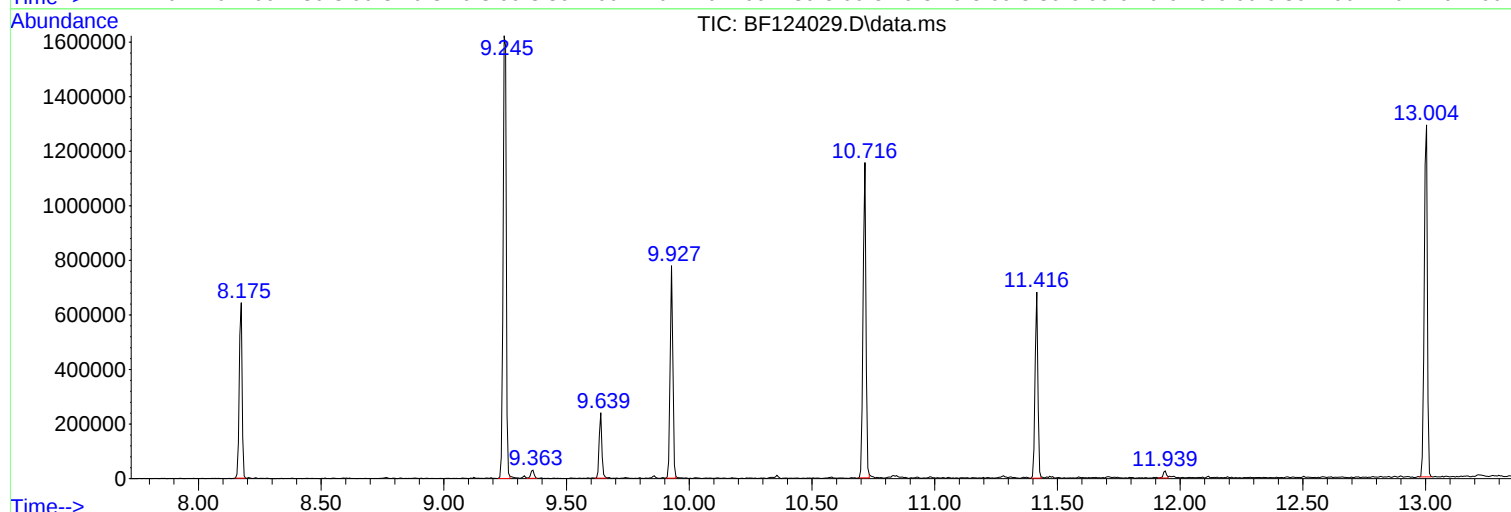
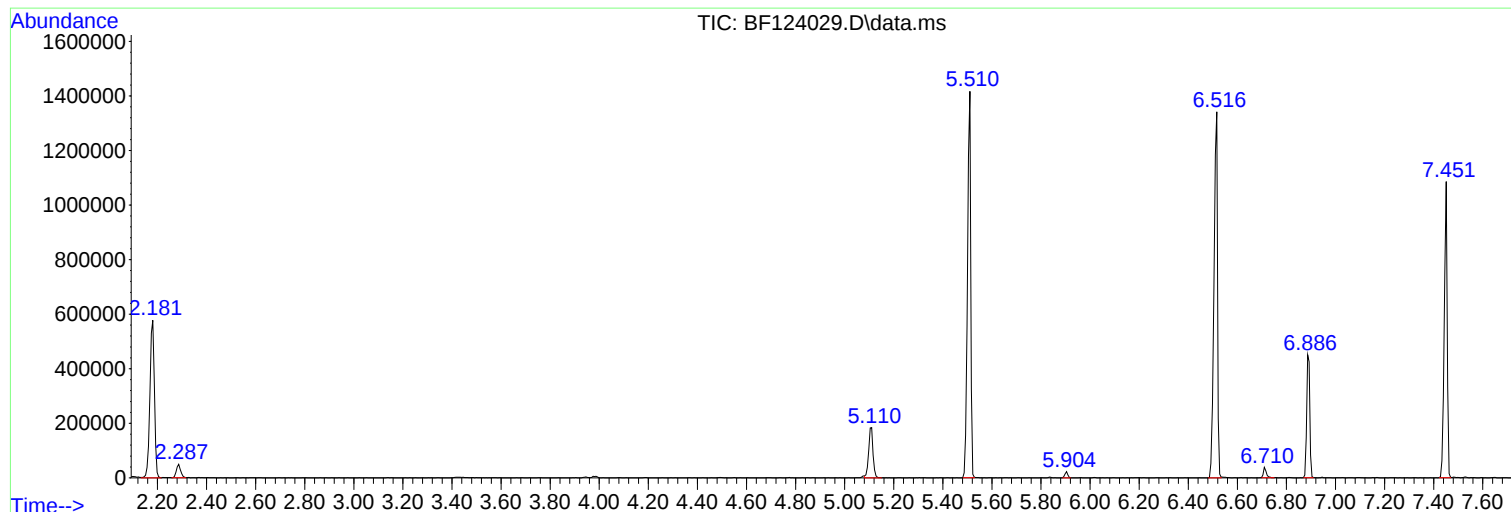
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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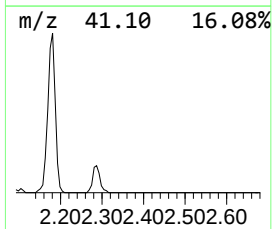
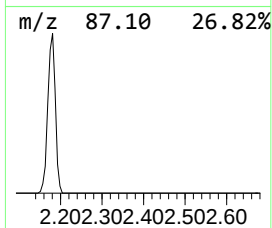
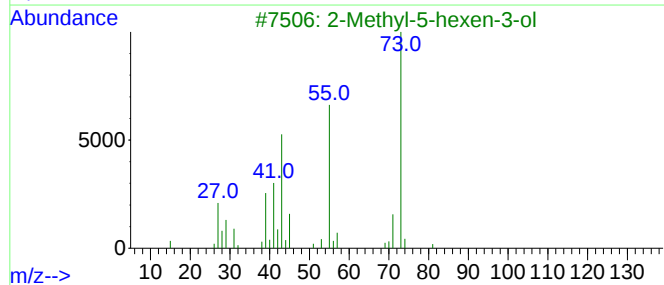
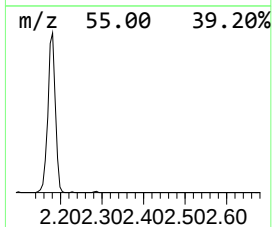
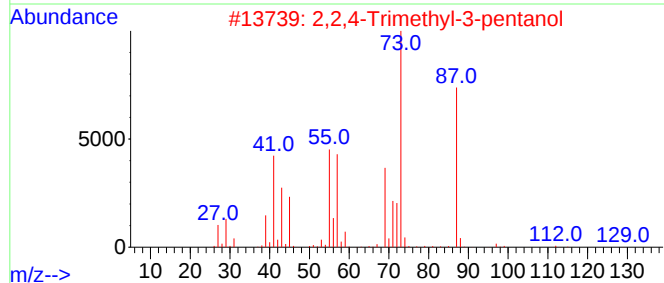
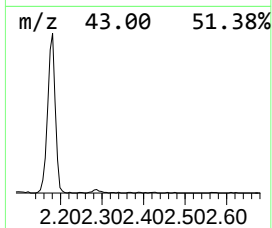
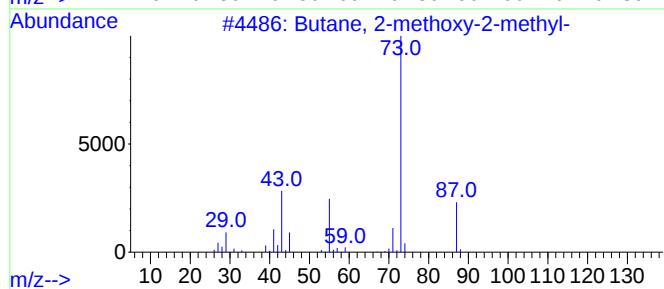
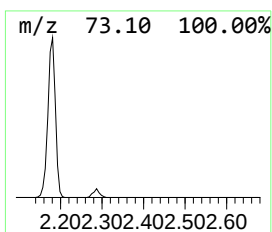
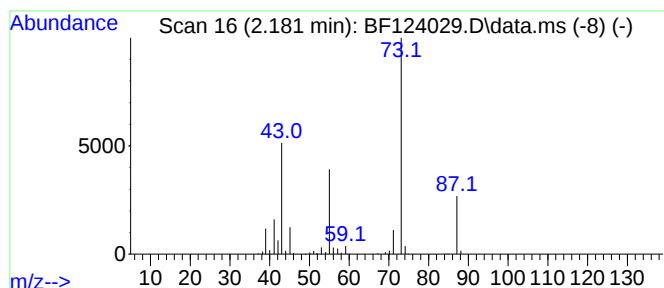
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	37.14 ng	736400	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	33
3			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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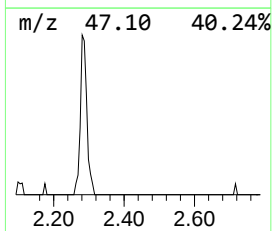
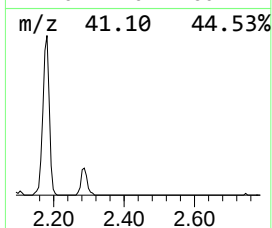
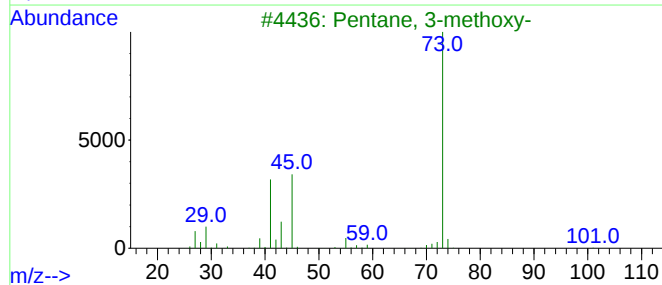
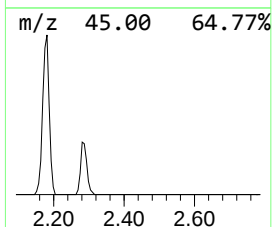
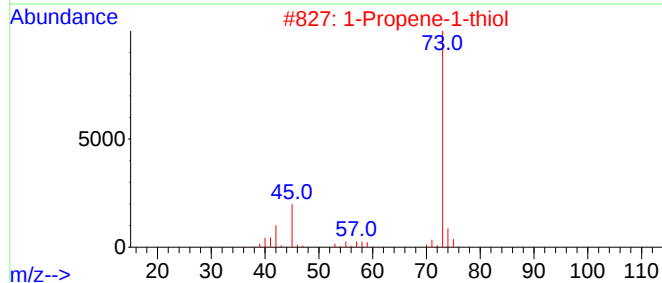
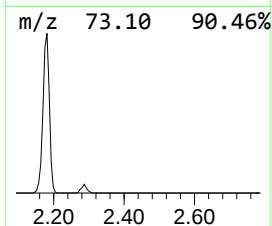
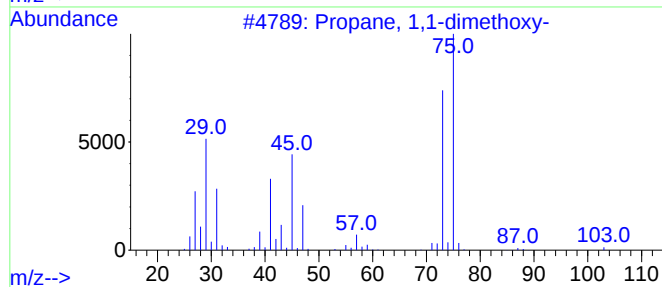
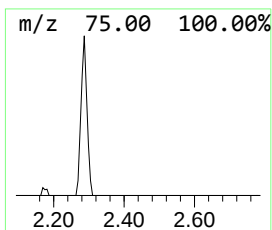
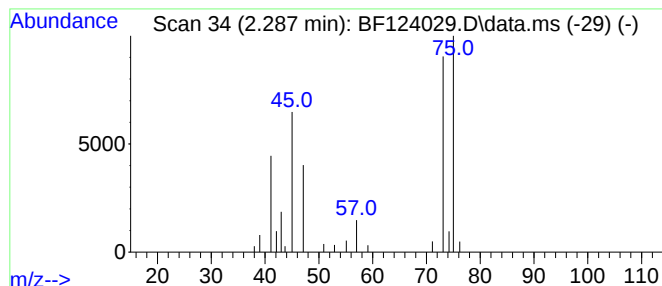
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.287	3.00 ng	59517	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2			1-Propene-1-thiol	74	C3H6S	000925-89-3	10
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
4			Trimethylene glycol monomethyl e...	90	C4H10O2	001589-49-7	9
5			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9



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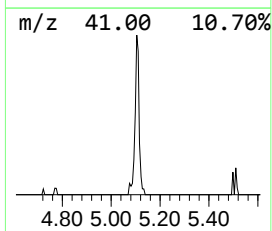
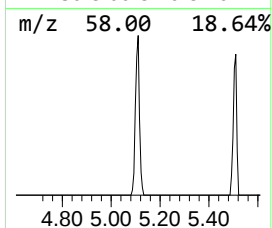
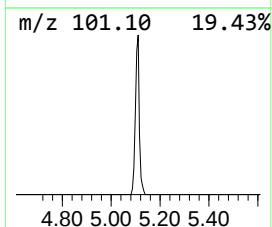
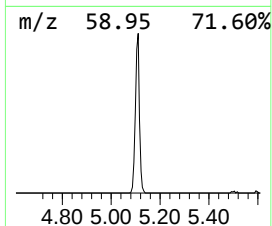
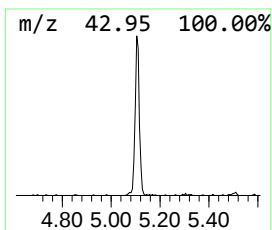
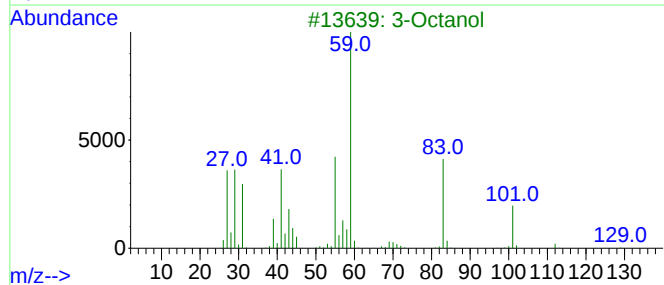
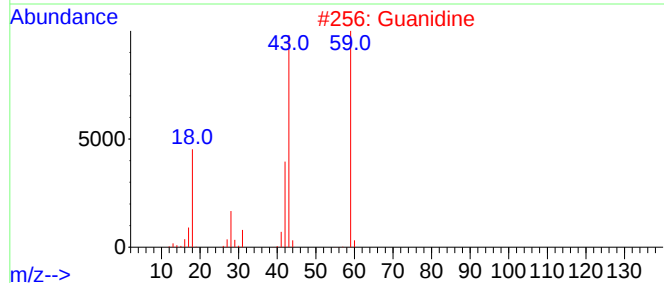
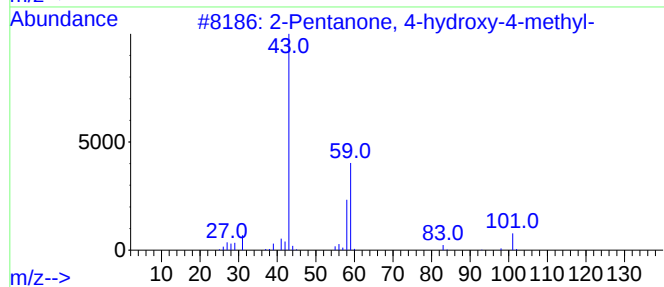
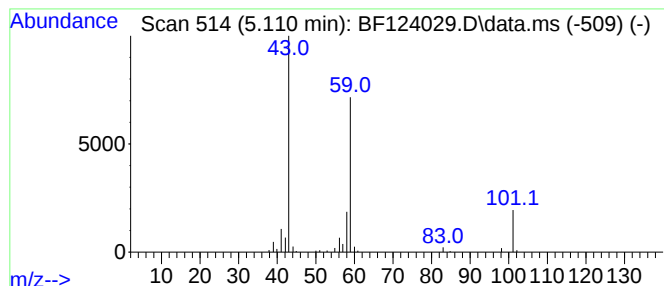
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	11.49 ng	227830	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Guanidine	59	CH5N3	000113-00-8	43		
3	3-Octanol	130	C8H18O	000589-98-0	33		
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23		



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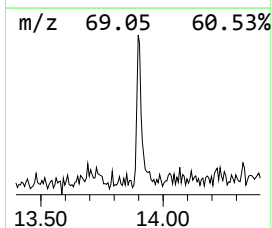
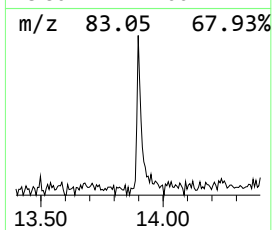
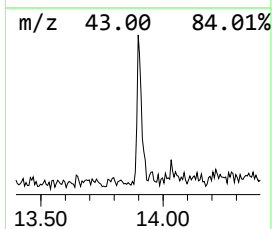
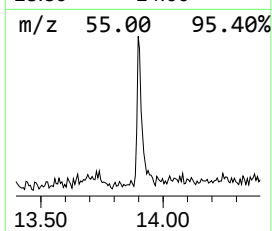
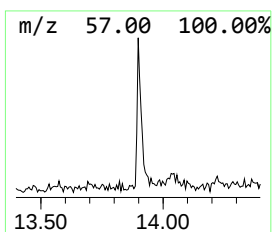
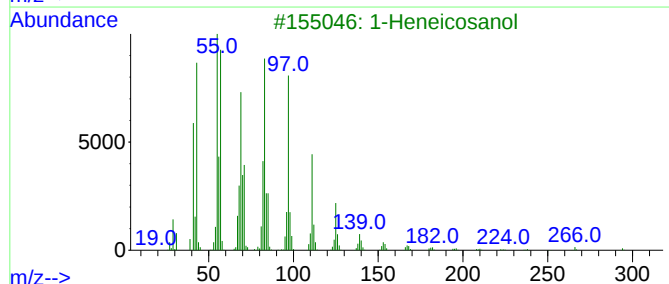
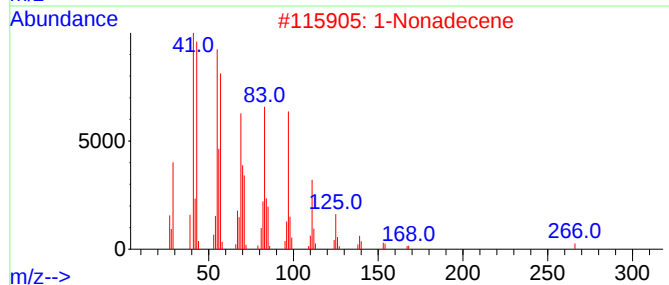
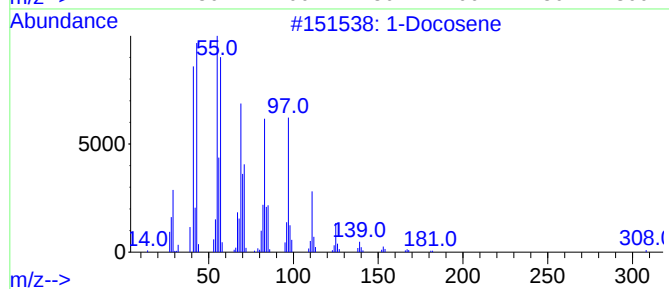
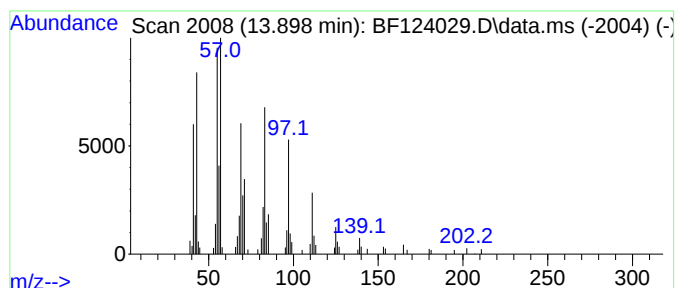
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	10.15 ng	210836	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	91
2	1-Nonadecene			266	C19H38	018435-45-5	91
3	1-Heneicosanol			312	C21H44O	015594-90-8	90
4	17-Pentatriacontene			491	C35H70	006971-40-0	90
5	Octacosanol			410	C28H58O	000557-61-9	87



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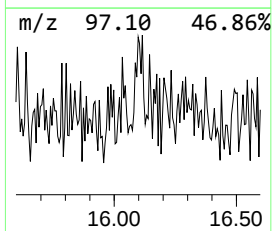
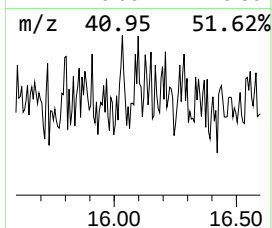
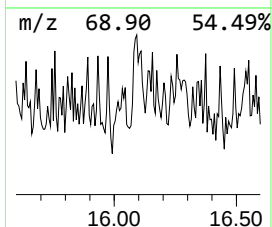
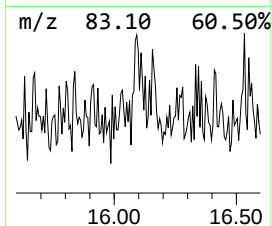
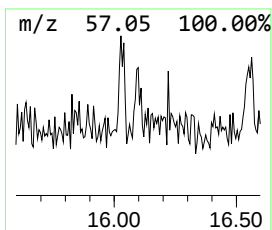
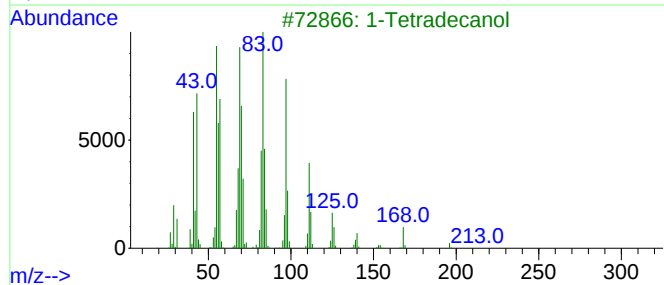
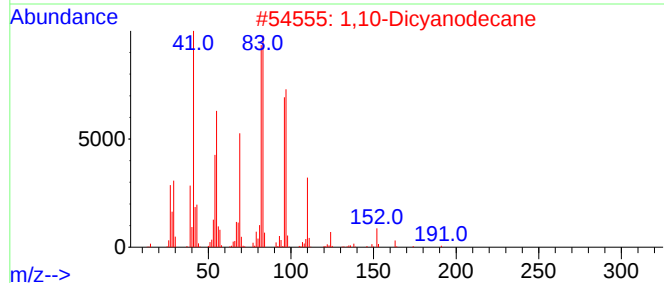
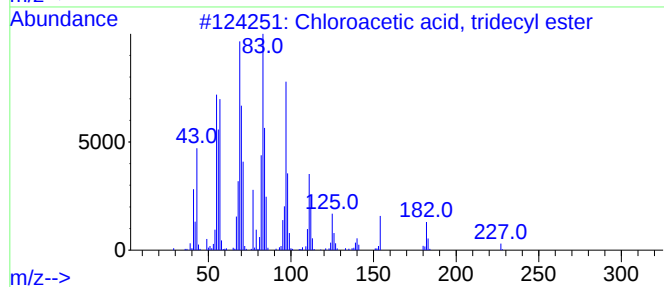
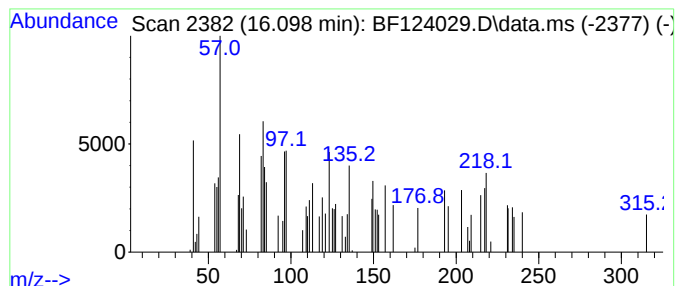
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 unknown16.098 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.098	2.13 ng	37784	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Chloroacetic acid, tridecyl ester	276	C15H29ClO2	018277-85-5	11
2			1,10-Dicyanodecane	192	C12H20N2	004543-66-2	10
3			1-Tetradecanol	214	C14H30O	000112-72-1	10
4			Acetic acid, trifluoro-, undecyl...	268	C13H23F3O2	053800-01-4	10
5			Chloroacetic acid, pentadecyl ester	304	C17H33ClO2	070301-47-2	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.181	37.1	ng	736400	1	6.892	396512	20.0
Propane, 1,1-di...	2.287	3.0	ng	59517	1	6.892	396512	20.0
2-Pentanone, 4-...	5.110	11.5	ng	227830	1	6.892	396512	20.0
1-Docosene	13.898	10.2	ng	210836	5	14.057	415271	20.0
unknown16.098	16.098	2.1	ng	37784	6	15.545	354749	20.0