

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021022\
 Data File : BF126850.D
 Acq On : 10 Feb 2022 18:23
 Operator : CG\JU
 Sample : N1359-02
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-9D

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-BF020922.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126850.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.551	415	419	422	rBV	1985284	1740237	41.98%	8.152%
2	5.822	461	465	469	rVB	84571	70913	1.71%	0.332%
3	6.551	584	589	598	rBV	1344417	1265682	30.54%	5.929%
4	6.940	651	655	658	rBV	899903	707518	17.07%	3.314%
5	6.993	660	664	672	rBV	53110	62741	1.51%	0.294%
6	7.504	743	751	754	rBV	2714686	2532380	61.10%	11.863%
7	8.222	869	873	876	rBV	1182110	943549	22.76%	4.420%
8	9.298	1051	1056	1059	rBV	4855516	4144969	100.00%	19.417%
9	9.369	1064	1068	1070	rVB	67406	58418	1.41%	0.274%
10	9.957	1162	1168	1169	rBV2	56962	58949	1.42%	0.276%
11	9.981	1169	1172	1175	rVB	1144820	1011829	24.41%	4.740%
12	10.075	1185	1188	1191	rBV	96599	72382	1.75%	0.339%
13	10.769	1302	1306	1309	rBV	2800725	2478659	59.80%	11.611%
14	10.875	1322	1324	1333	rVB4	35393	56979	1.37%	0.267%
15	11.469	1421	1425	1428	rBV	1300270	1046799	25.25%	4.904%
16	12.857	1659	1661	1669	rVB	207319	182897	4.41%	0.857%
17	13.057	1690	1695	1698	rBV	3800898	3584673	86.48%	16.793%
18	13.998	1849	1855	1856	rBV5	41037	64263	1.55%	0.301%
19	14.110	1871	1874	1878	rBV	746952	640968	15.46%	3.003%
20	14.427	1924	1928	1932	rBV	80252	74204	1.79%	0.348%
21	15.621	2126	2131	2139	rBV	430986	547619	13.21%	2.565%

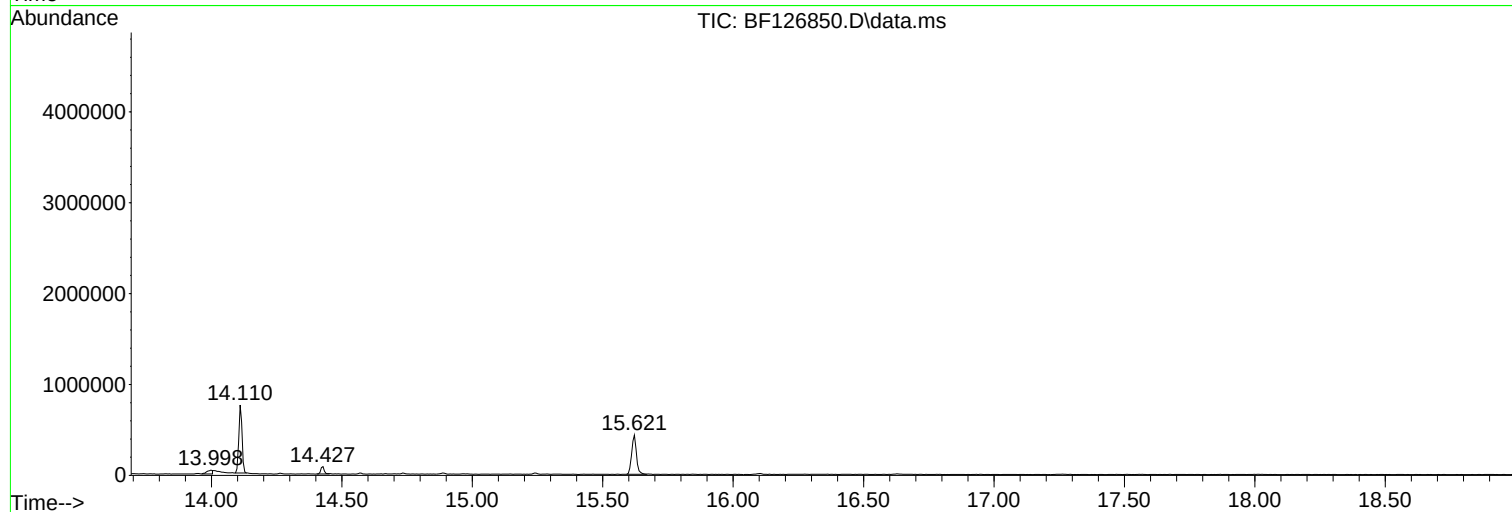
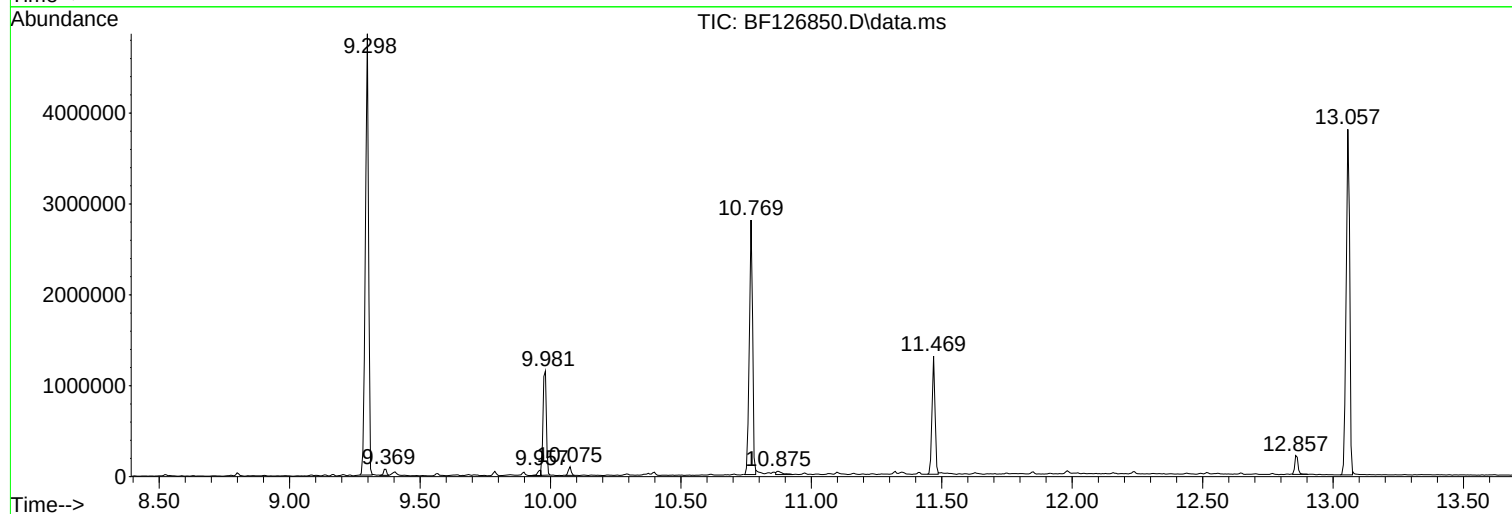
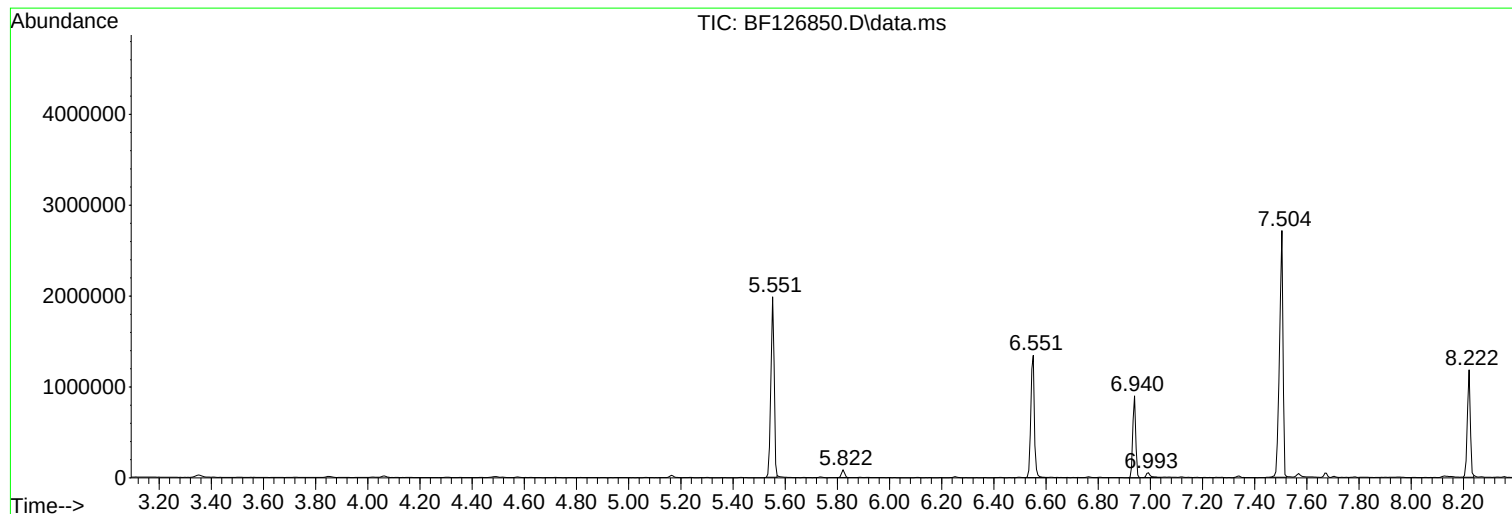
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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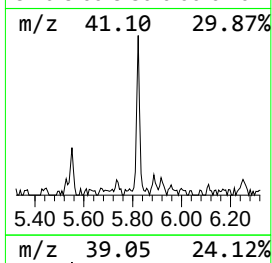
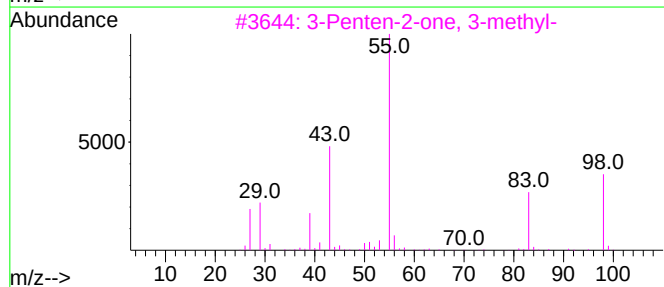
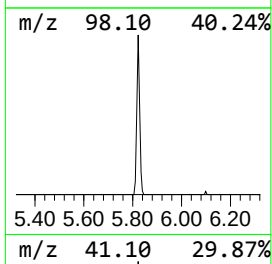
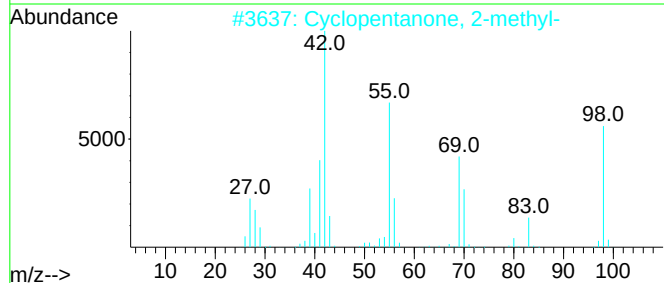
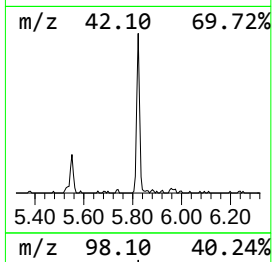
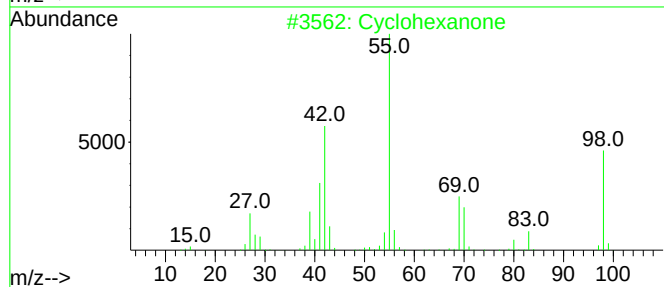
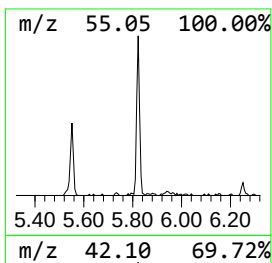
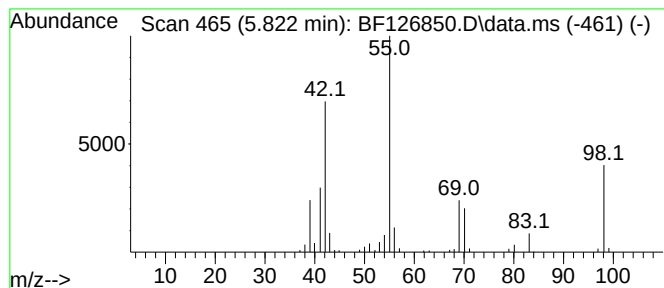
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020922.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Cyclohexanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.822	2.00 ng	70913	1,4-Dichlorobenzene-d4	6.940

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone	98	C6H10O	000108-94-1	91
2			Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	87
3			3-Penten-2-one, 3-methyl-	98	C6H10O	000565-62-8	38
4			2(3H)-Furanone, 5-methyl-	98	C5H6O2	000591-12-8	38
5			1-Pentene	70	C5H10	000109-67-1	38



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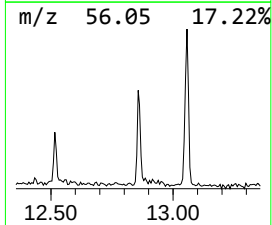
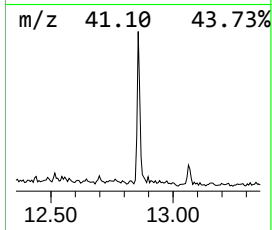
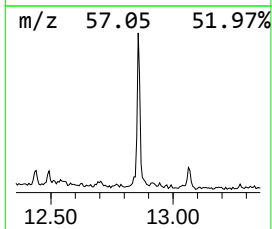
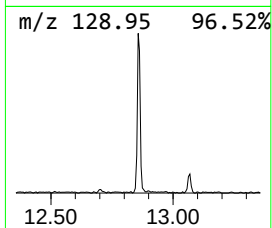
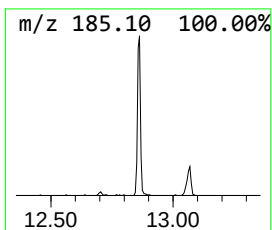
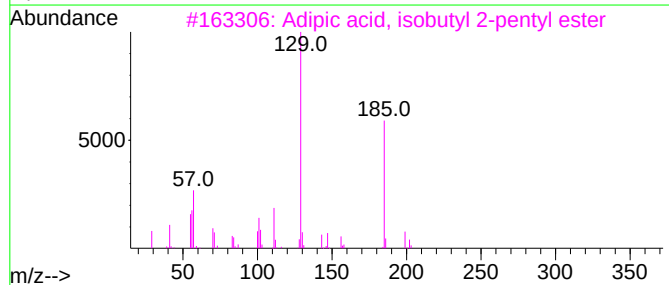
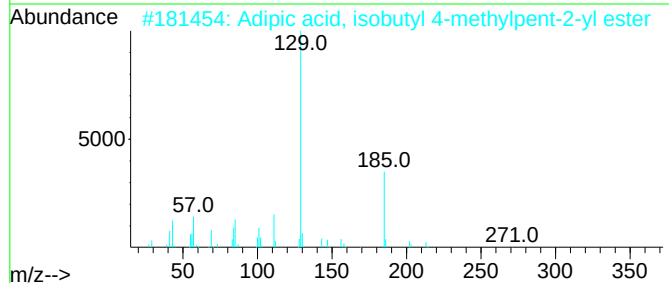
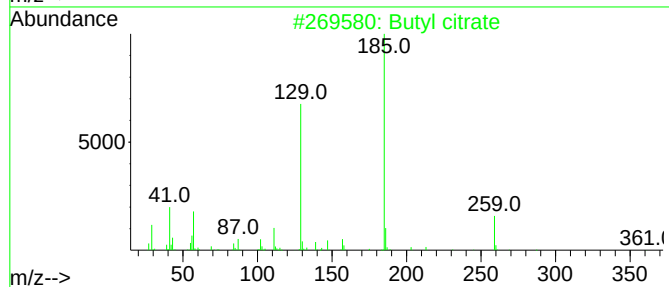
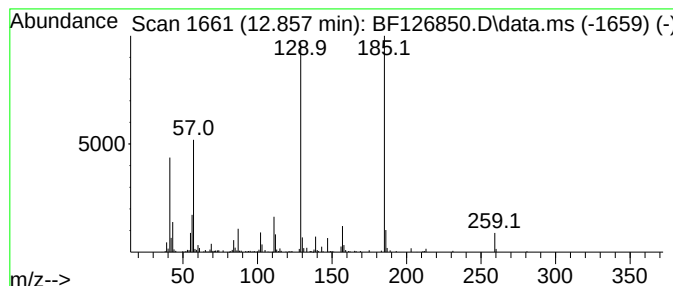
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020922.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butyl citrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.857	5.71 ng	182897	Chrysene-d12	14.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl citrate	360	C18H32O7	000077-94-1	86
2			Adipic acid, isobutyl 4-methylpe...	286	C16H30O4	1000353-50-1	72
3			Adipic acid, isobutyl 2-pentyl e...	272	C15H28O4	1000324-15-6	72
4			Hexanedioic acid, bis(2-methylpr...	258	C14H26O4	000141-04-8	72
5			Adipic acid, 4-heptyl isobutyl e...	300	C17H32O4	1000349-73-6	72



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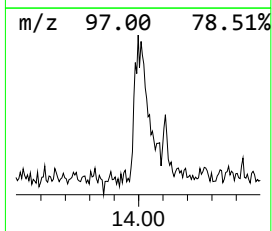
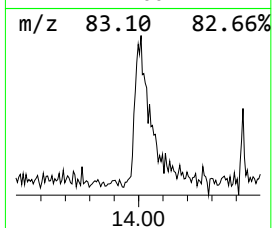
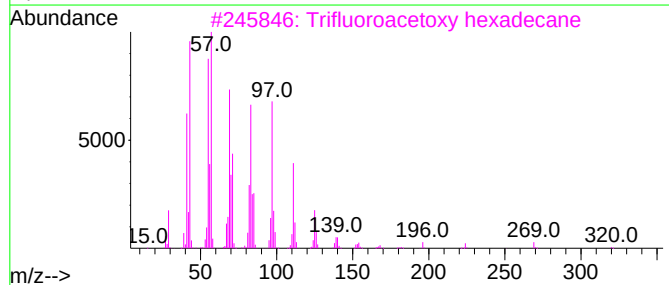
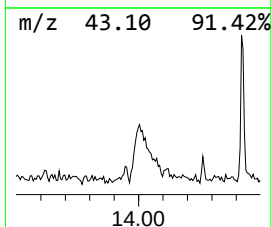
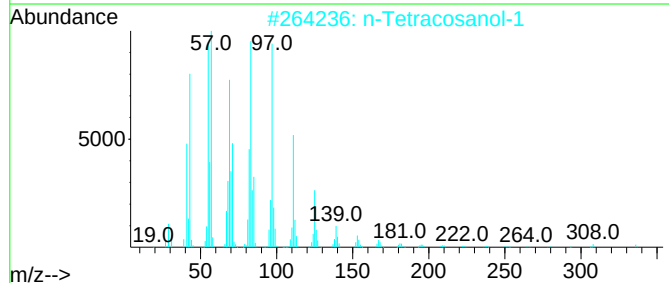
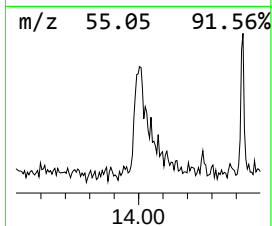
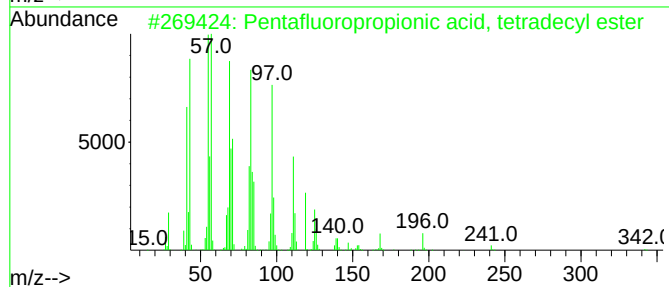
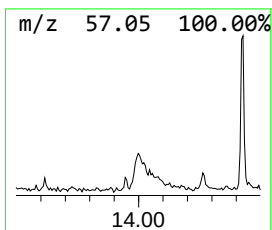
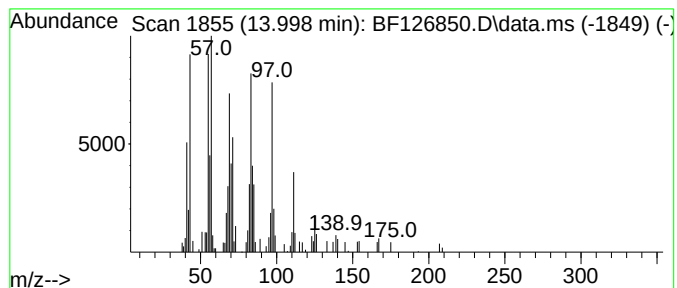
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.998	2.01 ng	64263	Chrysene-d12	14.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	94
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4			Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	91
5			3-Eicosene, (E)-	280	C20H40	074685-33-9	91



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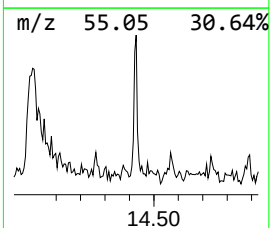
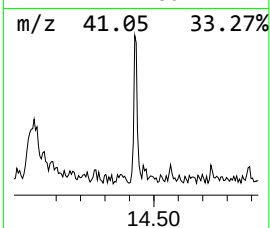
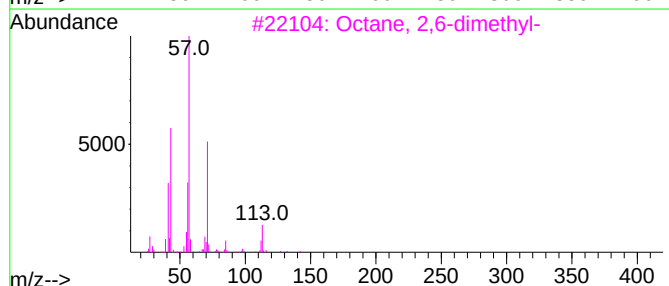
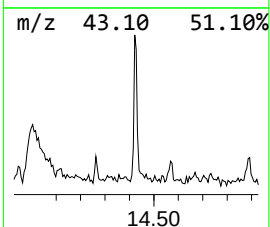
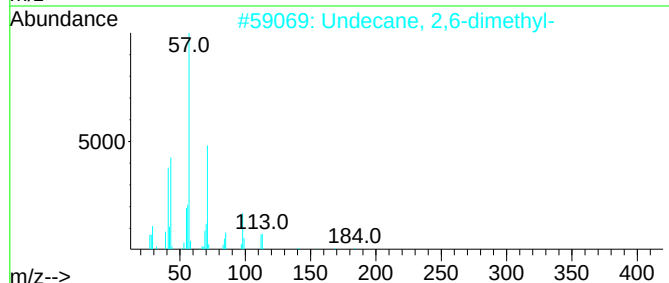
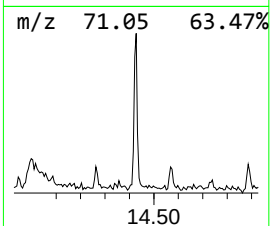
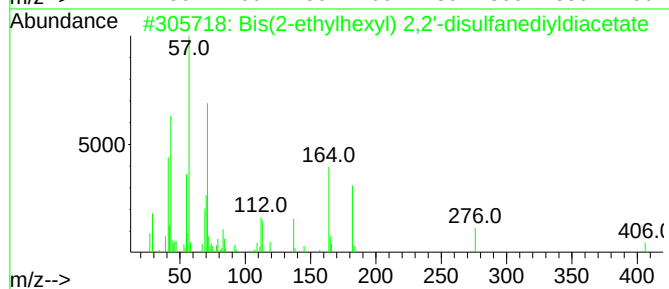
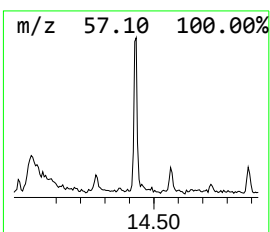
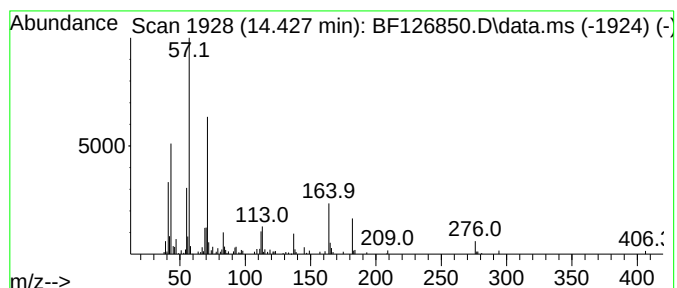
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Bis(2-ethylhexyl) 2,2'-disu... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.427	2.32 ng	74204	Chrysene-d12	14.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bis(2-ethylhexyl) 2,2'-disulfane...	406	C20H38O4S2	062268-47-7	60
2			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	49
3			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	47
4			Tridecane, 5-propyl-	226	C16H34	055045-11-9	47
5			Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	47



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TIC Library : C:\Database\NIST0.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexanone	5.822	2.0	ng	70913	1	6.940	707518	20.0
Butyl citrate	12.857	5.7	ng	182897	5	14.110	640968	20.0
Pentafluoroprop...	13.998	2.0	ng	64263	5	14.110	640968	20.0
Bis(2-ethylhexy...	14.427	2.3	ng	74204	5	14.110	640968	20.0