

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062623\
 Data File : BF133967.D
 Acq On : 26 Jun 2023 23:16
 Operator : CG\JU
 Sample : 03365-33
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP3

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-BF062623.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133967.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	4	11	17	rBV	1211025	1620819	65.57%	8.428%
2	2.269	27	31	38	rVB2	29842	41288	1.67%	0.215%
3	5.099	508	512	519	rVB	146082	181287	7.33%	0.943%
4	5.493	574	579	582	rBV	2549568	2306444	93.30%	11.993%
5	6.493	744	749	752	rBV	2531720	2374325	96.05%	12.346%
6	6.851	807	810	814	rBV	939570	747987	30.26%	3.889%
7	7.416	901	906	909	rBV	1711179	1453529	58.80%	7.558%
8	8.134	1024	1028	1031	rBV	1001134	861463	34.85%	4.479%
9	9.210	1207	1211	1214	rBV	3101743	2472039	100.00%	12.854%
10	9.892	1323	1327	1330	rBV	907497	797976	32.28%	4.149%
11	10.604	1445	1448	1452	rBV	423135	357545	14.46%	1.859%
12	10.680	1457	1461	1465	rBV	1472620	1361577	55.08%	7.080%
13	10.916	1498	1501	1508	rVB	55656	45537	1.84%	0.237%
14	11.386	1577	1581	1584	rBV	888246	798638	32.31%	4.153%
15	11.910	1667	1670	1675	rBV	87634	95450	3.86%	0.496%
16	12.980	1848	1852	1856	rBV	2745883	2471629	99.98%	12.852%
17	13.886	2002	2006	2014	rBV	248868	329693	13.34%	1.714%
18	14.045	2029	2033	2038	rBV	576998	533628	21.59%	2.775%
19	15.551	2285	2289	2294	rVB	305391	380882	15.41%	1.980%

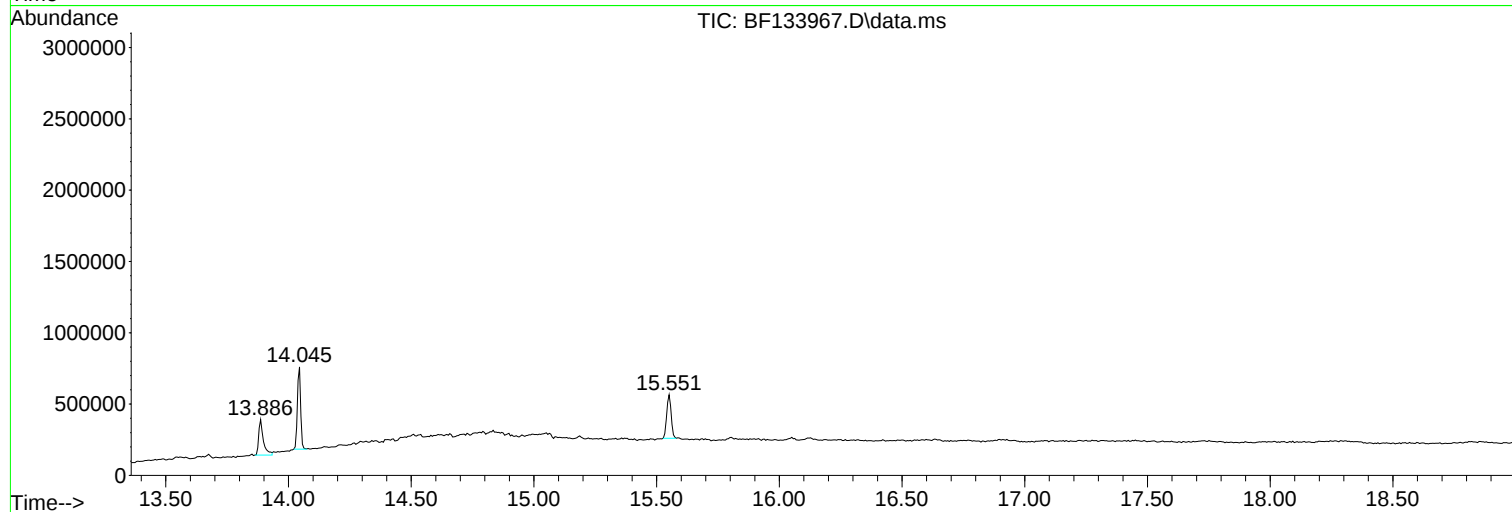
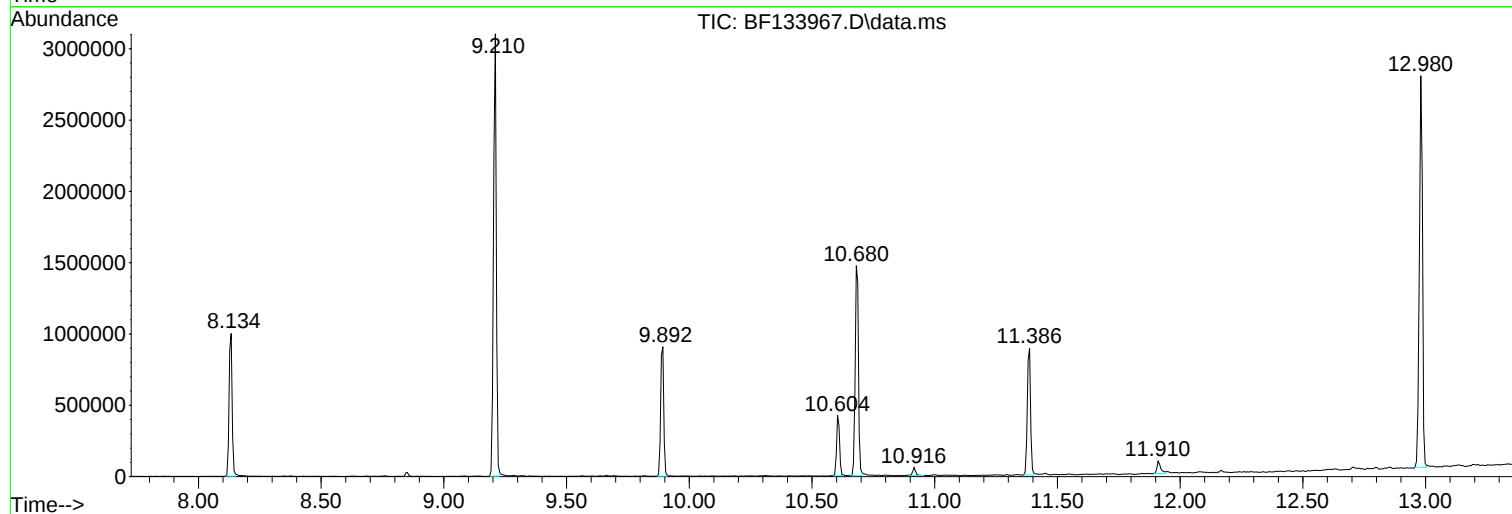
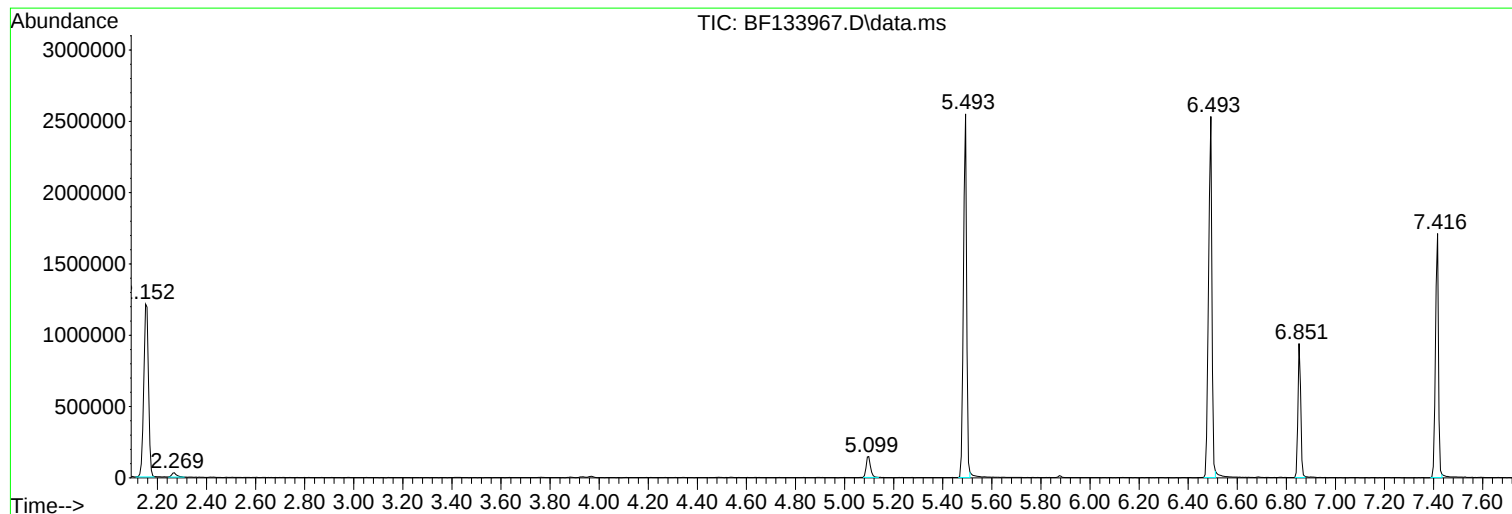
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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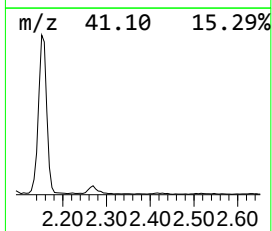
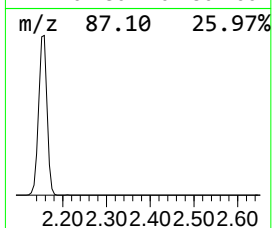
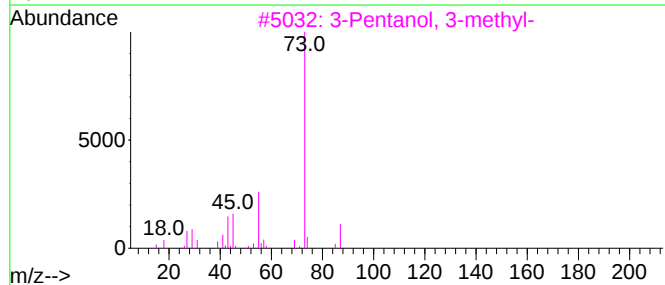
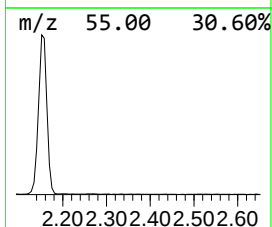
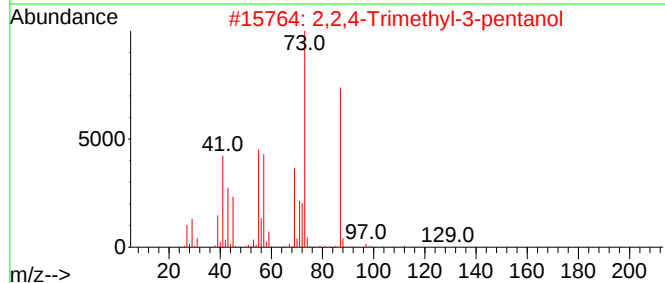
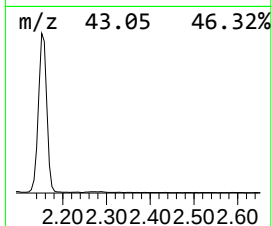
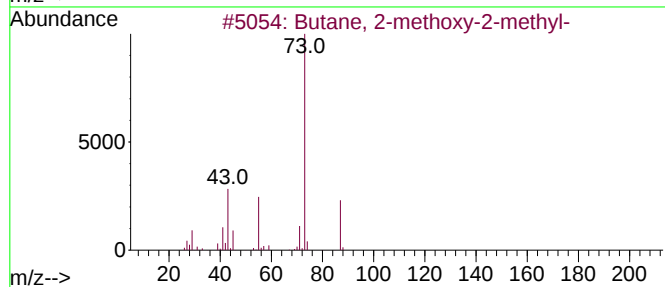
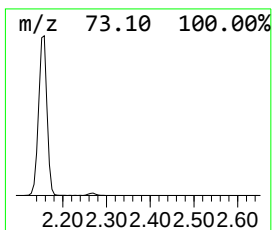
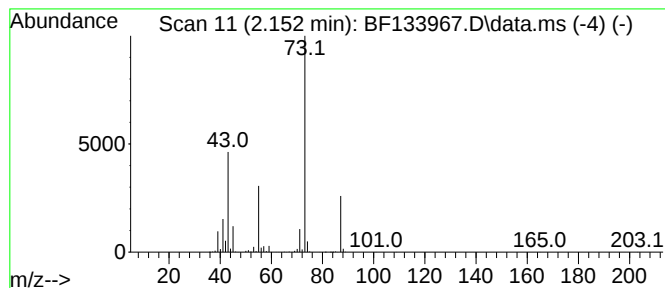
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.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.
2.152	43.34 ng	1620820	1,4-Dichlorobenzene-d4	6.851

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	39
3			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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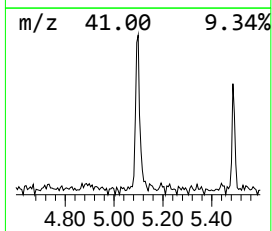
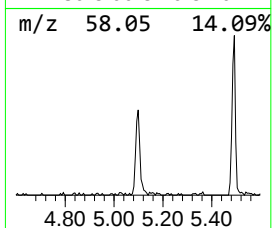
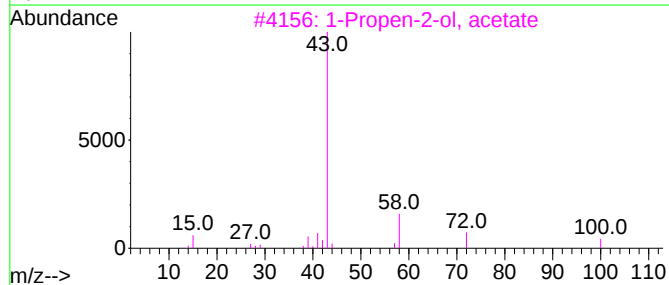
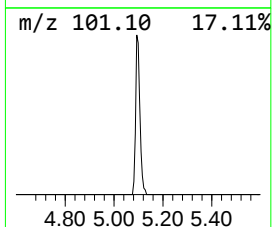
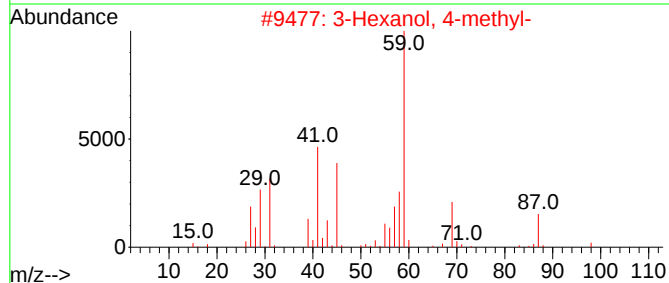
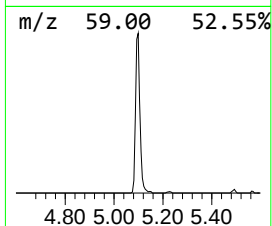
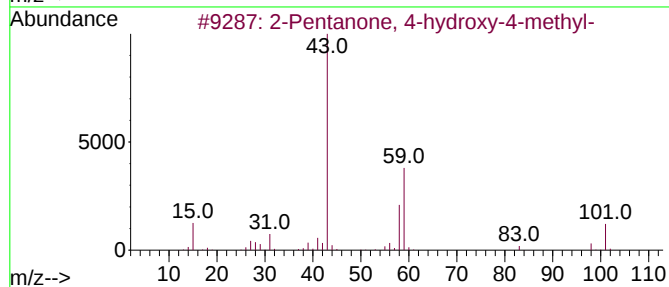
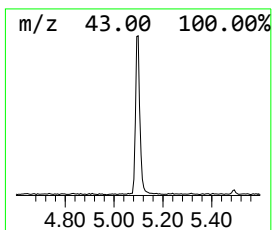
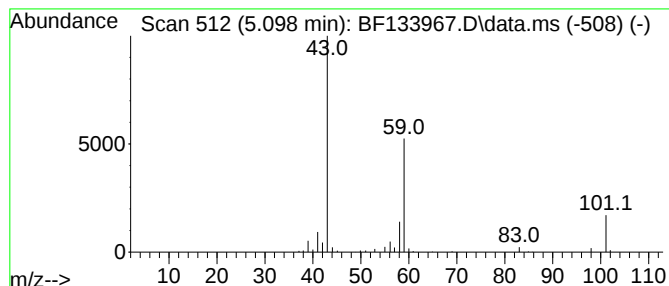
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	4.85 ng	181287	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9
5			Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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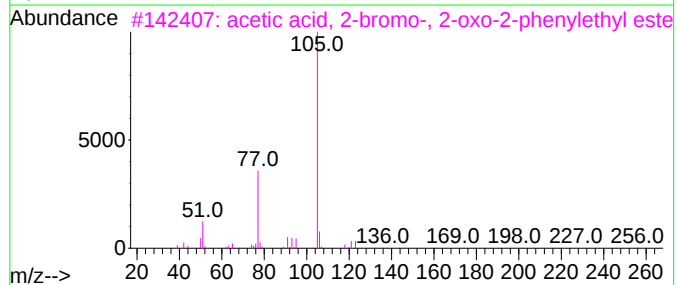
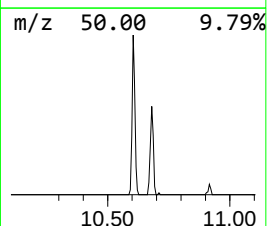
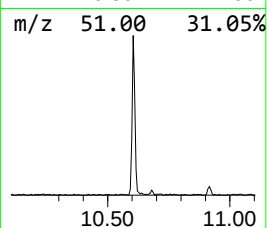
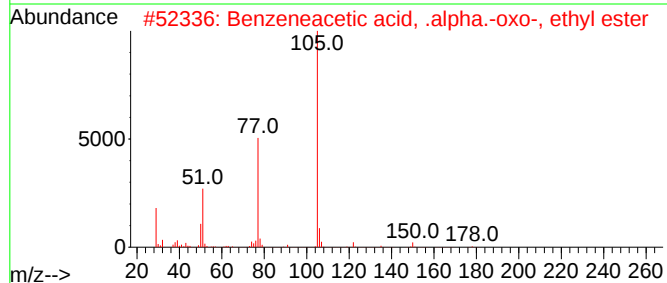
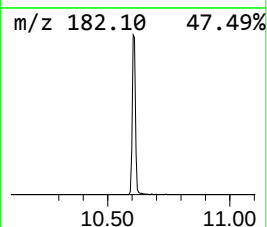
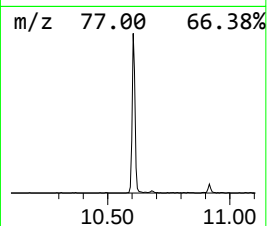
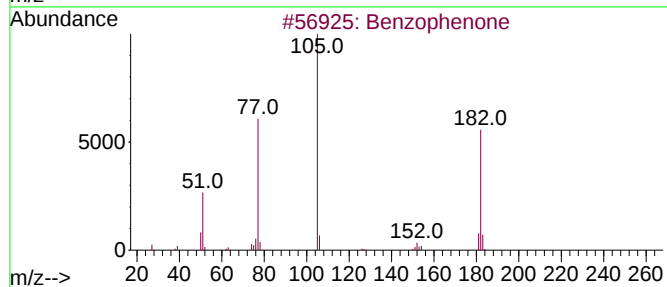
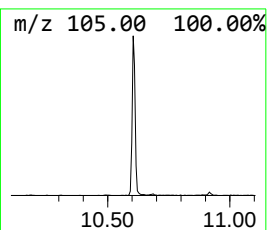
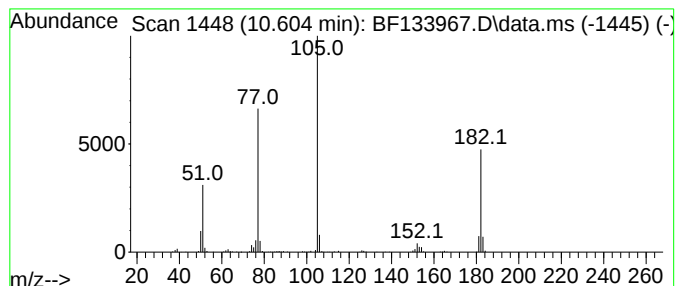
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.604	8.96 ng	357545	Acenaphthene-d10	9.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzeneacetic acid, .alpha.-oxo-...	178	C10H10O3	001603-79-8	50
3			acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	50
4			Methyl 2-benzoyl-4-cyanobutanoate	231	C13H13NO3	1010486-83-8	50
5			Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	50



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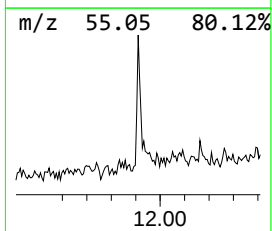
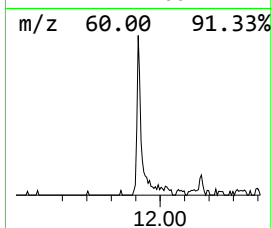
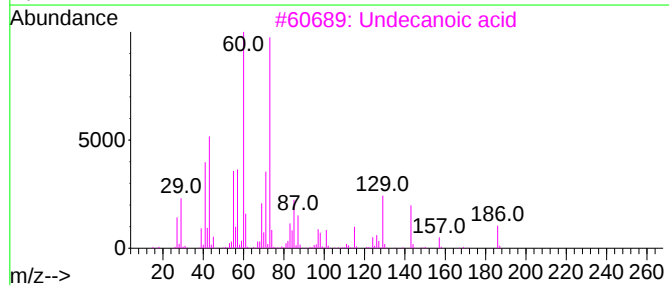
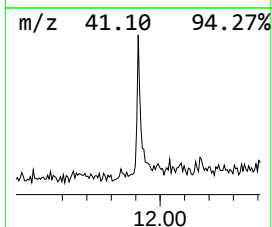
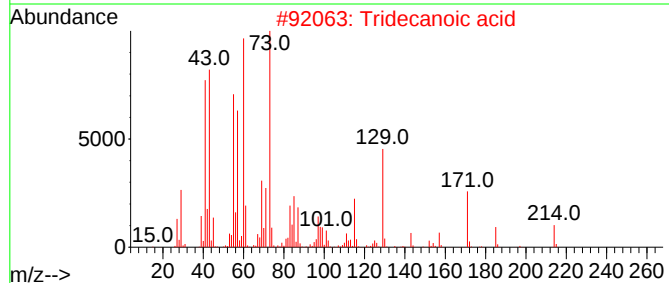
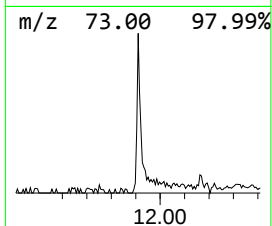
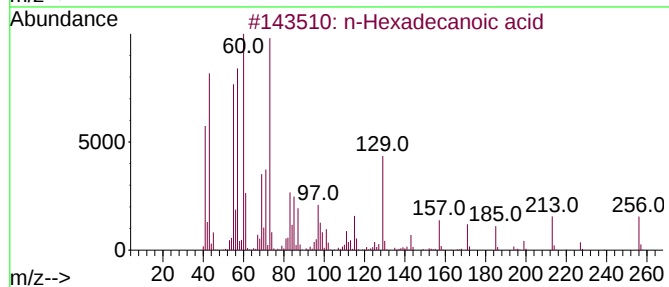
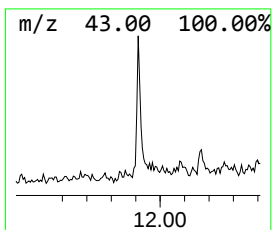
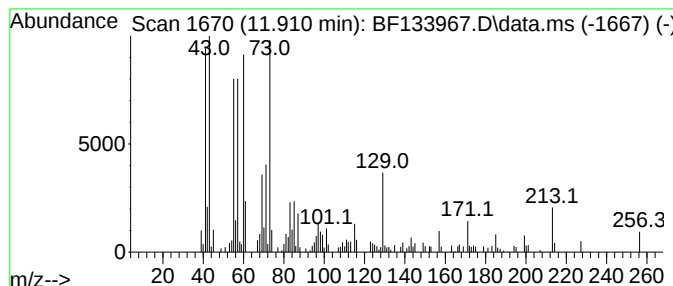
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	2.39 ng	95450	Phenanthrene-d10	11.386

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		Undecanoic acid	186	C11H22O2	000112-37-8	76
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	74



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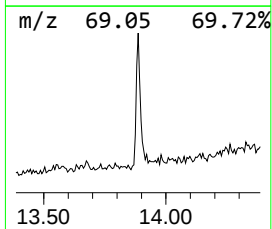
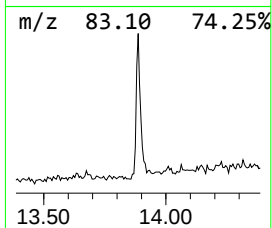
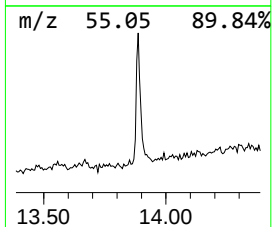
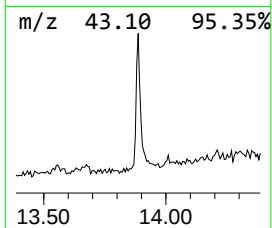
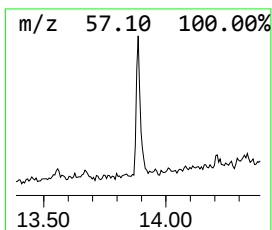
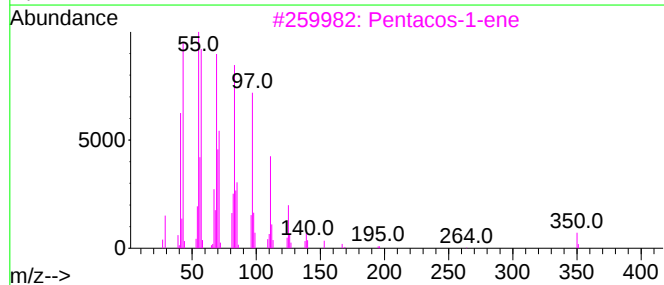
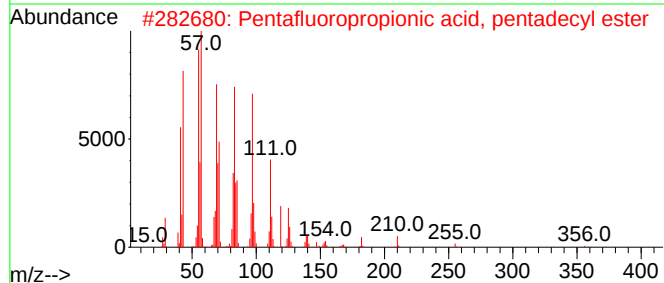
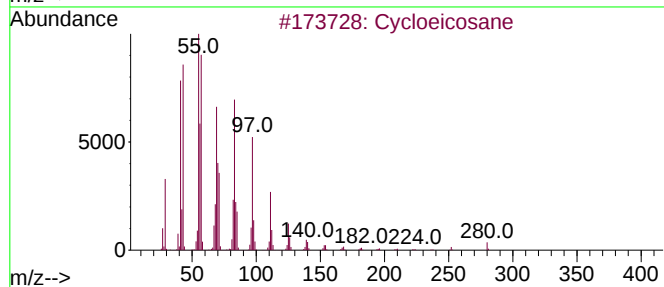
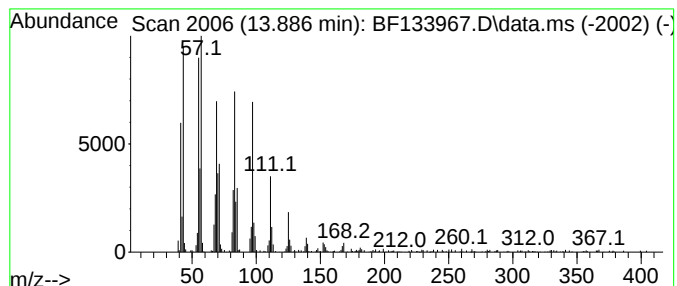
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Peak Number 5 Cycloeicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	12.36 ng	329693	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloeicosane	280	C20H40	000296-56-0	95
2			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3			Pentacos-1-ene	350	C25H50	016980-85-1	94
4			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.152	43.3	ng	1620820	1	6.851	747987	20.0
2-Pentanone, 4-...	5.098	4.8	ng	181287	1	6.851	747987	20.0
Benzophenone	10.604	9.0	ng	357545	3	9.892	797976	20.0
n-Hexadecanoic ...	11.910	2.4	ng	95450	4	11.386	798638	20.0
Cycloeicosane	13.886	12.4	ng	329693	5	14.045	533628	20.0