

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061323\
 Data File : BF133740.D
 Acq On : 13 Jun 2023 20:07
 Operator : CG\JU
 Sample : 03136-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ELI-SUB-LD-CON

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-BF060923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133740.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.504	234	241	248	rVB	51059	81377	2.17%	0.598%
2	4.422	389	397	401	rBV	2547479	3742310	100.00%	27.483%
3	5.051	496	504	507	rBV	1759711	2426768	64.85%	17.822%
4	5.440	566	570	576	rBV	219387	198027	5.29%	1.454%
5	6.457	739	743	749	rBV	719840	630420	16.85%	4.630%
6	6.834	803	807	810	rBV	599689	527021	14.08%	3.870%
7	7.392	898	902	905	rBV	916588	721995	19.29%	5.302%
8	8.116	1021	1025	1028	rBV	626092	488802	13.06%	3.590%
9	9.186	1204	1207	1211	rBV	1285831	1093011	29.21%	8.027%
10	9.869	1320	1323	1327	rBV	617404	484036	12.93%	3.555%
11	10.581	1441	1444	1450	rVB	60778	46371	1.24%	0.341%
12	11.357	1572	1576	1580	rBV	695971	578772	15.47%	4.250%
13	12.945	1842	1846	1850	rBV	1633126	1416276	37.84%	10.401%
14	13.845	1996	1999	2014	rBV3	132415	260456	6.96%	1.913%
15	14.004	2023	2026	2030	rVB	648816	567698	15.17%	4.169%
16	15.468	2270	2275	2278	rBV	302122	353307	9.44%	2.595%

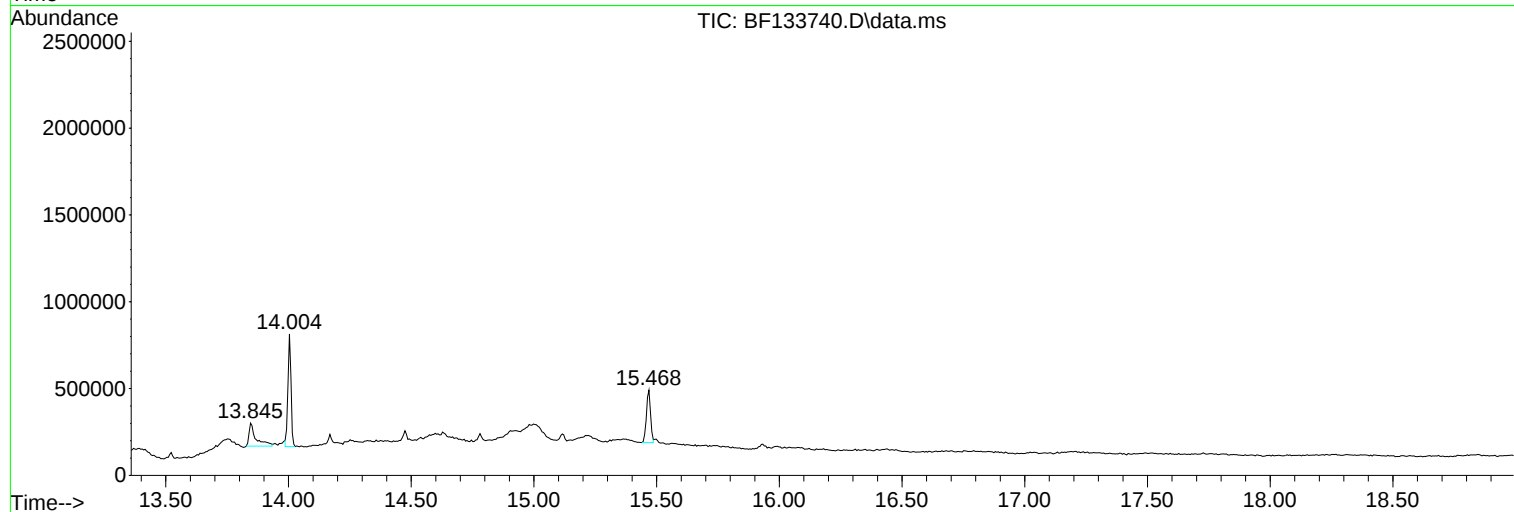
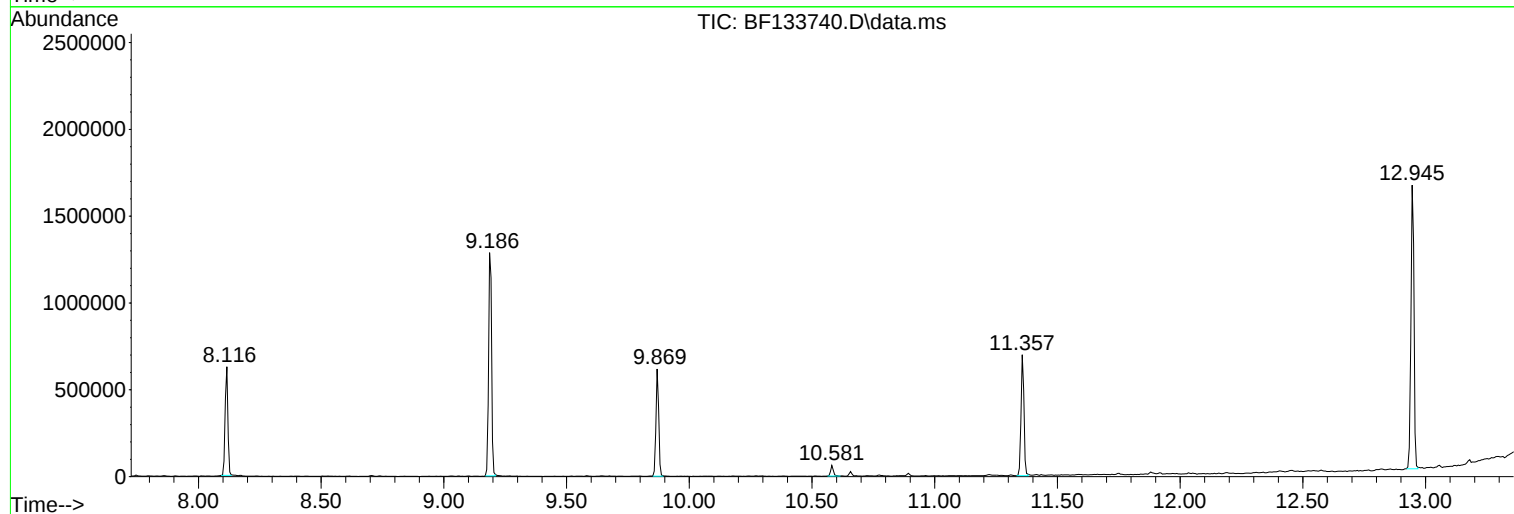
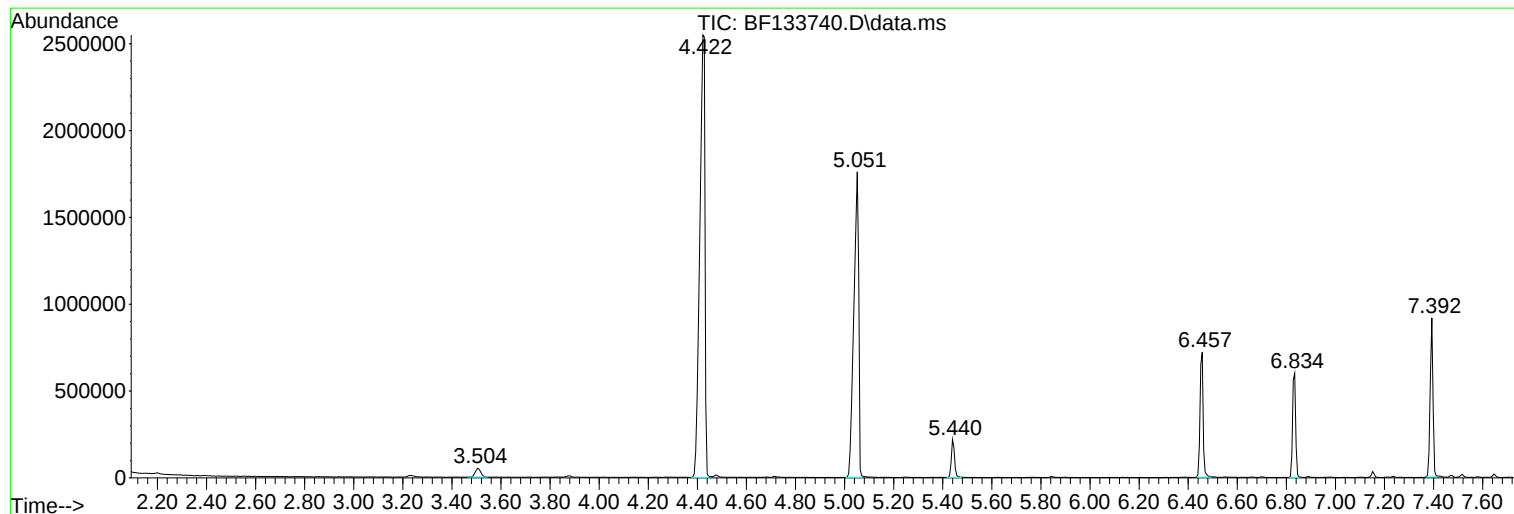
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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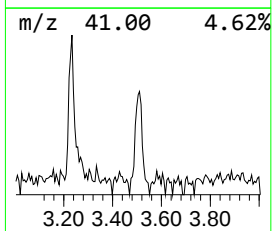
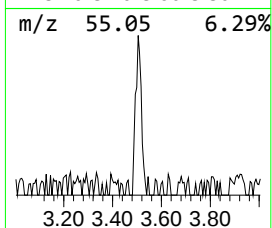
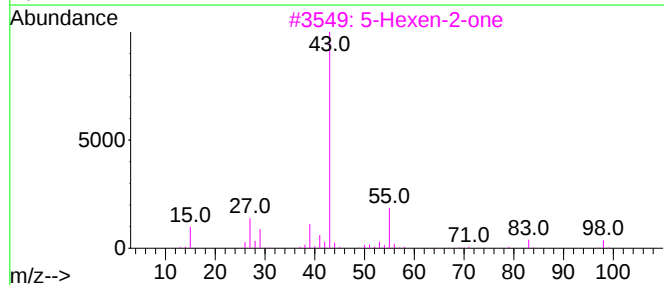
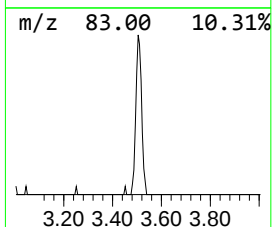
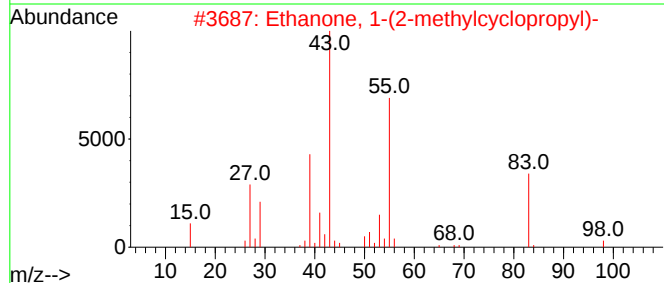
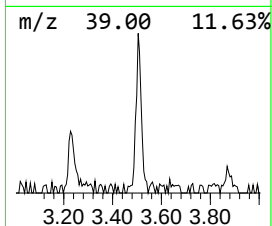
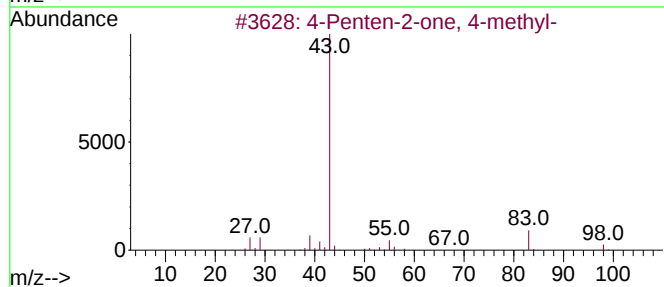
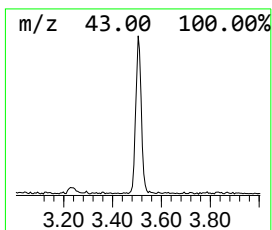
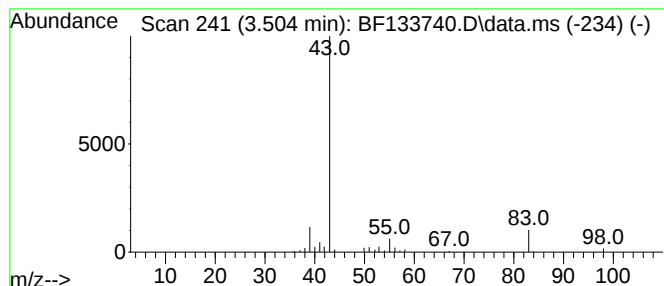
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.504	3.09 ng	81377	1,4-Dichlorobenzene-d4	6.834

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	72
2		Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	38
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		4-Hexen-2-one	98	C6H10O	025659-22-7	9
5		4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	9



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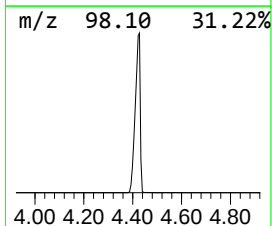
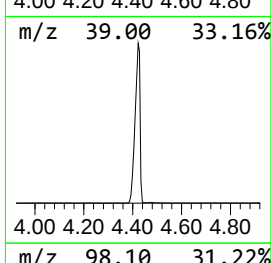
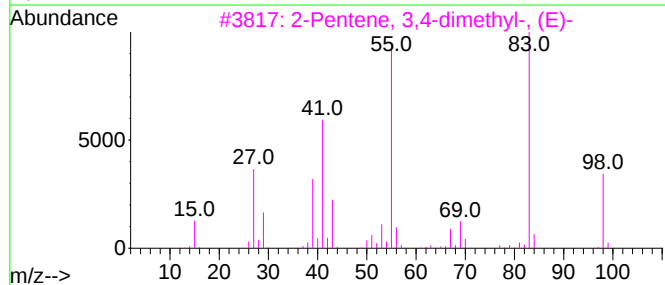
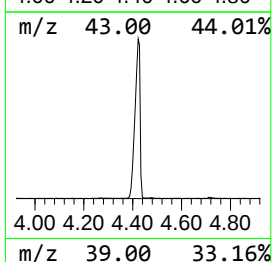
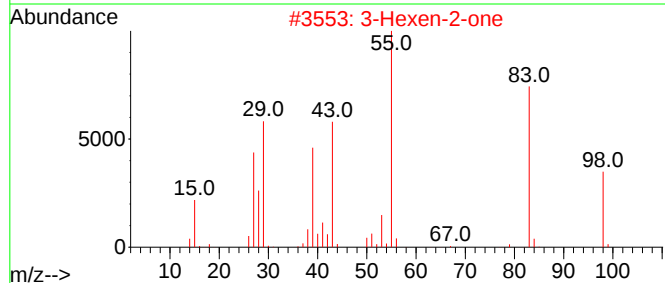
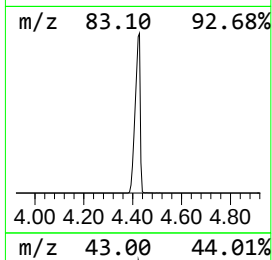
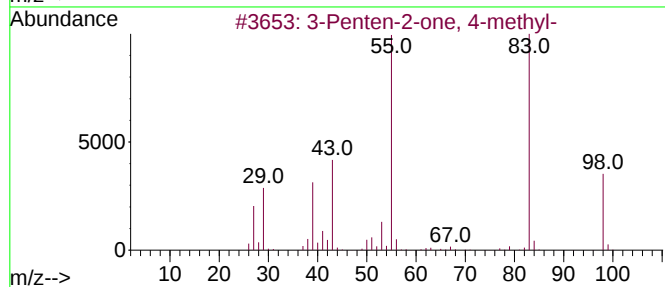
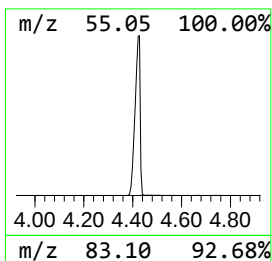
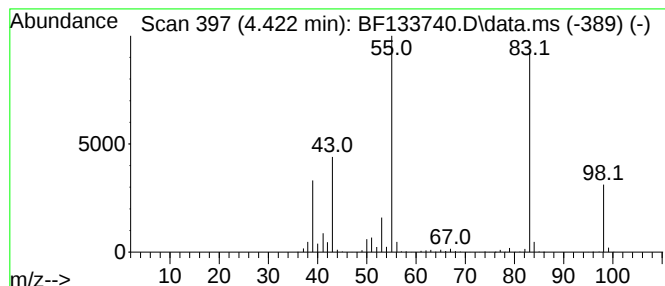
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.422	142.02 ng	3742310	1,4-Dichlorobenzene-d4	6.834

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78



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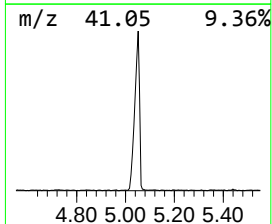
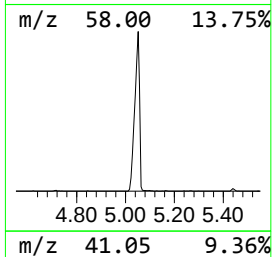
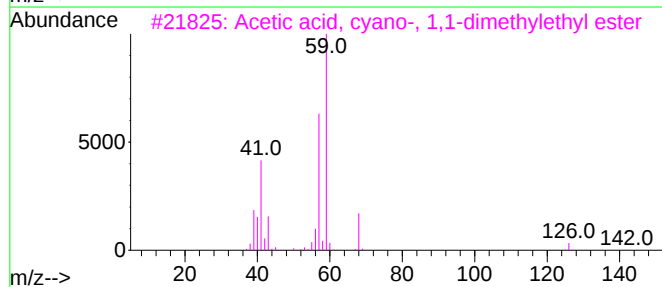
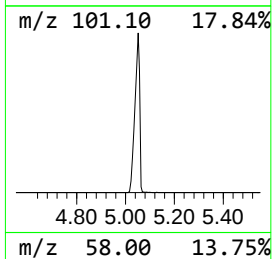
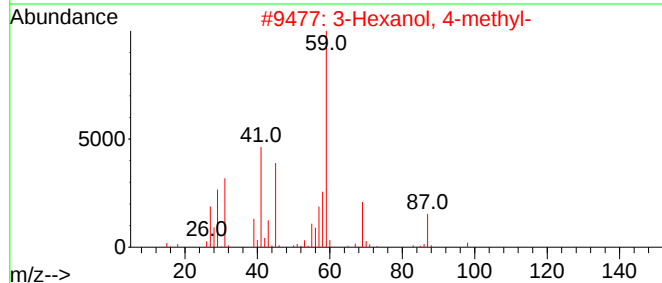
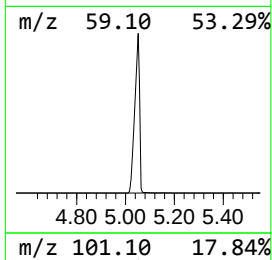
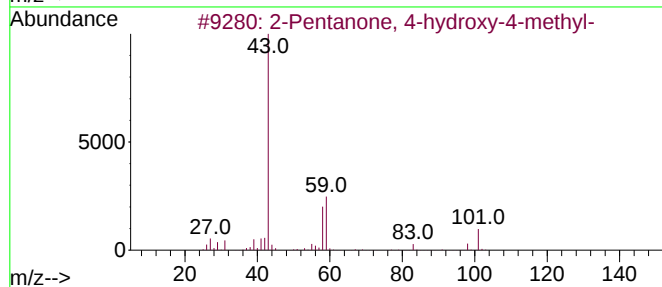
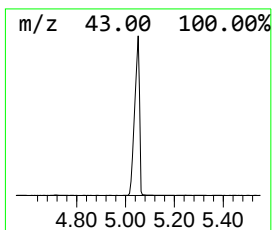
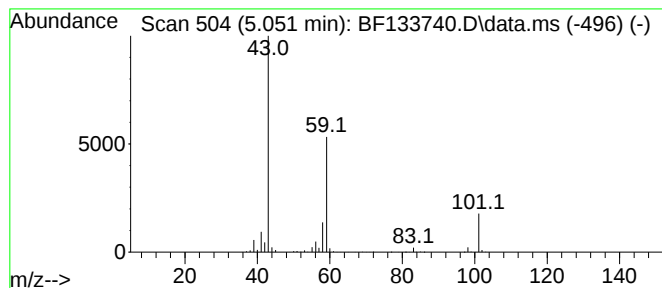
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.051	92.09 ng	2426770	1,4-Dichlorobenzene-d4	6.834

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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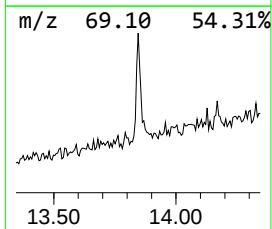
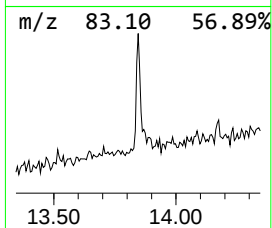
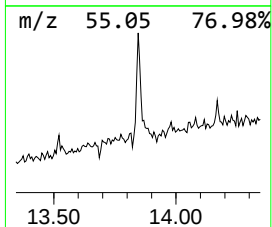
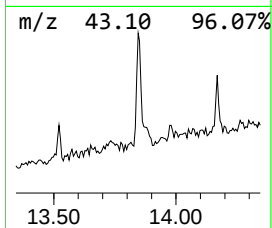
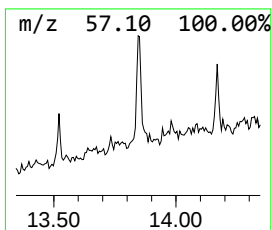
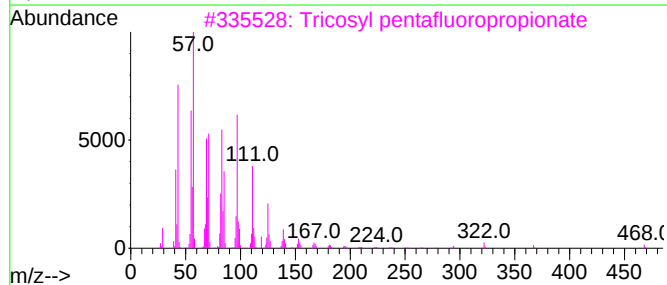
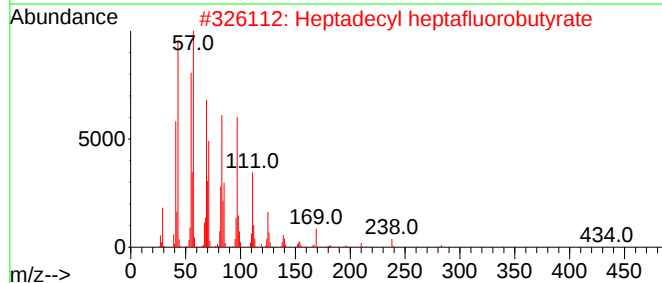
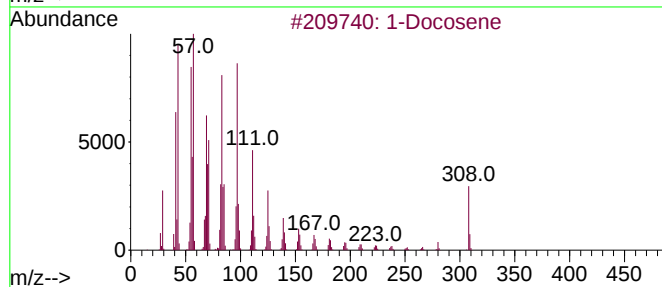
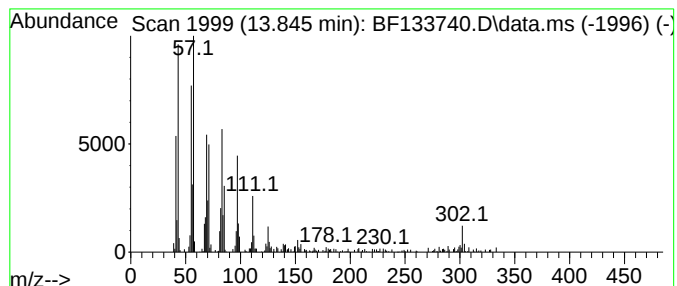
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Peak Number 4 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	9.18 ng	260456	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	97
2	Heptadecyl heptafluorobutyrate			452	C21H35F7O2	959085-66-6	93
3	Tricosyl pentafluoropropionate			486	C26H47F5O2	1000351-81-0	90
4	Tricosyl heptafluorobutyrate			536	C27H47F7O2	1000351-83-4	90
5	Nonadecyl pentafluoropropionate			430	C22H39F5O2	1000351-88-8	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Penten-2-one,...	3.504	3.1	ng	81377	1	6.834	527021	20.0
3-Penten-2-one,...	4.422	142.0	ng	3742310	1	6.834	527021	20.0
2-Pentanone, 4-...	5.051	92.1	ng	2426770	1	6.834	527021	20.0
1-Docosene	13.845	9.2	ng	260456	5	14.004	567698	20.0