

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121220\
 Data File : BF122679.D
 Acq On : 12 Dec 2020 15:37
 Operator : JU/CG
 Sample : L5042-08
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 KENS-B6-121020-13-15

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-BF120520.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122679.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	6	9	24	rVB	64568	115835	2.40%	0.380%
2	3.346	211	214	231	rBV	49775	103163	2.14%	0.339%
3	5.463	569	574	577	rBV	3646215	3649565	75.65%	11.981%
4	6.469	740	745	768	rBV	3257611	4001105	82.93%	13.136%
5	6.669	776	779	791	rBV	45487	62720	1.30%	0.206%
6	6.834	804	807	811	rBV	1047595	825400	17.11%	2.710%
7	7.398	898	903	906	rBV	2418655	2463319	51.06%	8.087%
8	8.116	1021	1025	1042	rVB	1066547	1093317	22.66%	3.589%
9	9.198	1203	1209	1212	rBV	4633113	4563094	94.58%	14.981%
10	9.586	1271	1275	1284	rBV	242899	226585	4.70%	0.744%
11	9.875	1319	1324	1327	rBV	1438685	1268678	26.30%	4.165%
12	10.663	1453	1458	1472	rBV	2836853	2663188	55.20%	8.743%
13	11.357	1572	1576	1584	rBV	1354029	1307587	27.10%	4.293%
14	11.886	1662	1666	1671	rBV	66566	91111	1.89%	0.299%
15	12.675	1795	1800	1811	rBV	178397	269626	5.59%	0.885%
16	12.951	1841	1847	1850	rBV	4795245	4824401	100.00%	15.838%
17	13.863	1996	2002	2021	rBV2	208700	680112	14.10%	2.233%
18	13.998	2021	2025	2033	rVB	1281532	1165931	24.17%	3.828%
19	15.463	2268	2274	2287	rBV	766810	997942	20.69%	3.276%
20	16.039	2363	2372	2376	rBV8	28149	87486	1.81%	0.287%

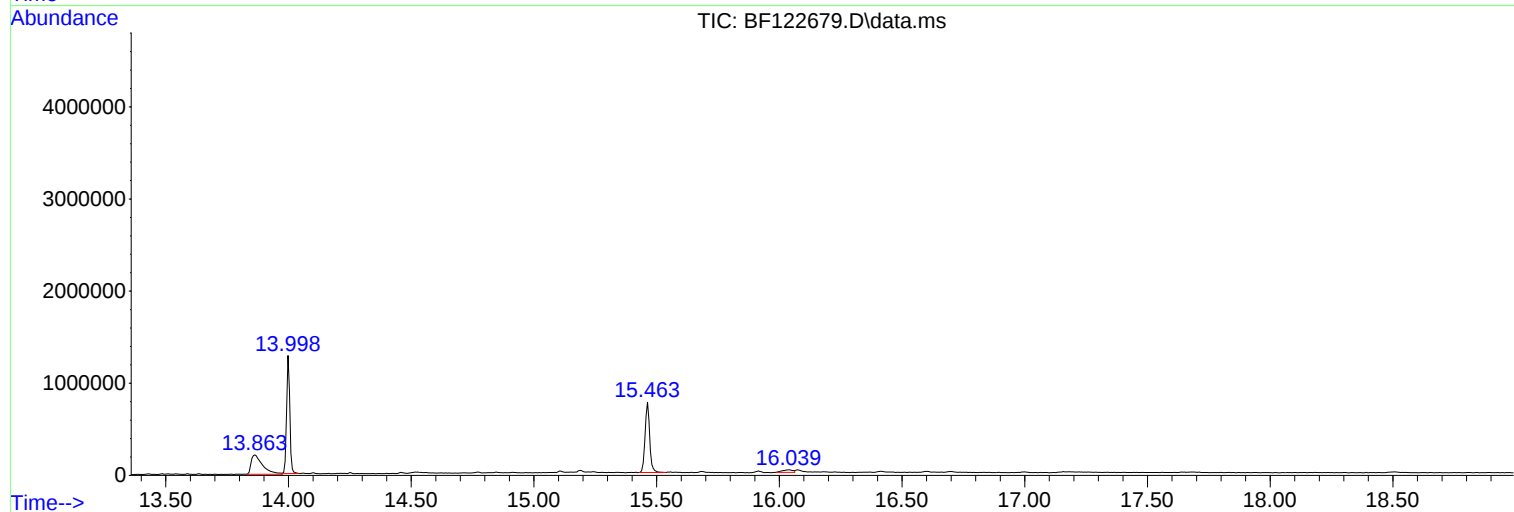
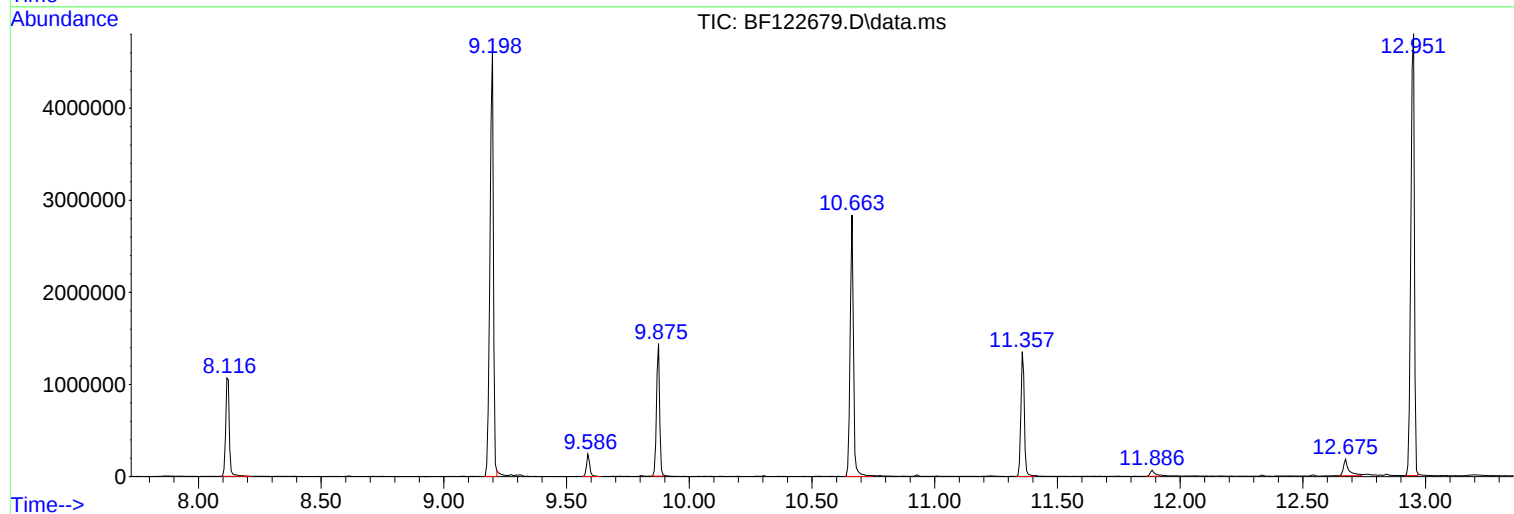
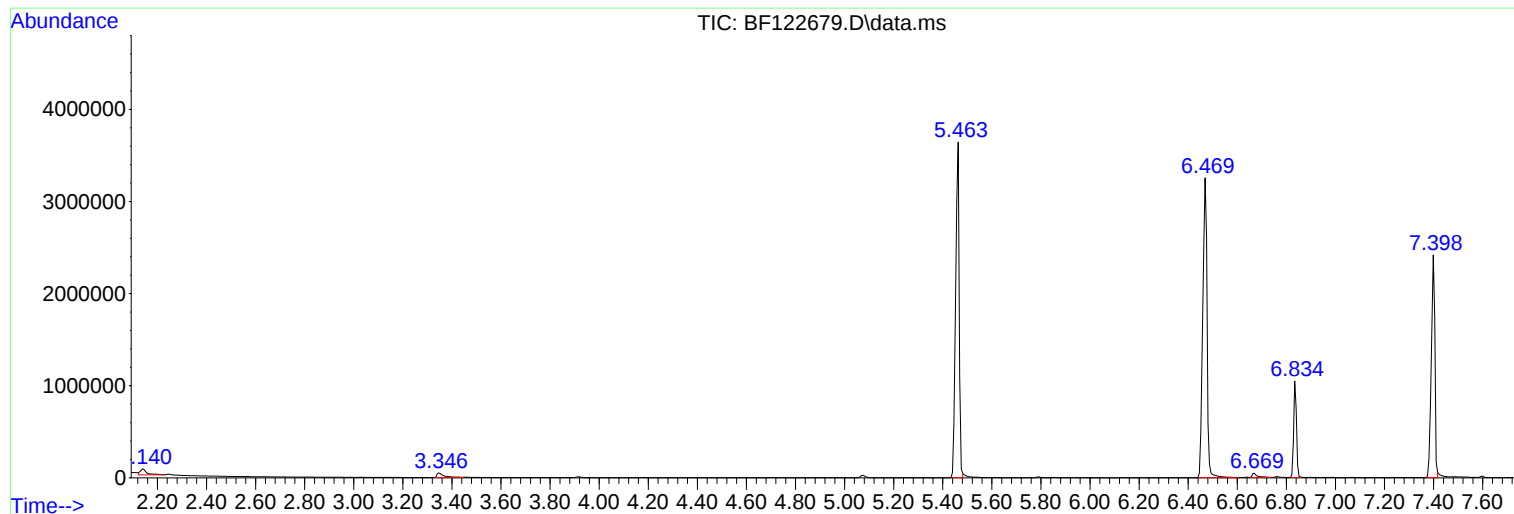
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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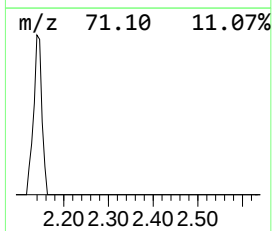
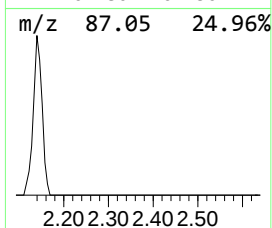
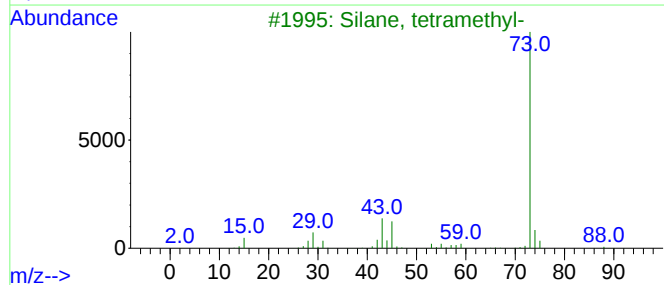
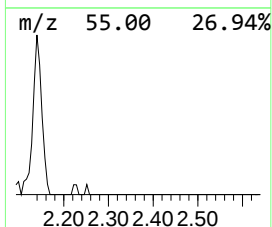
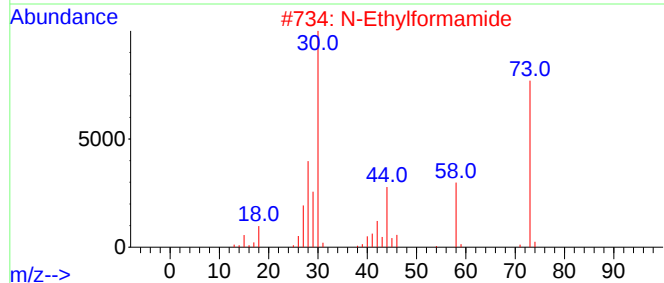
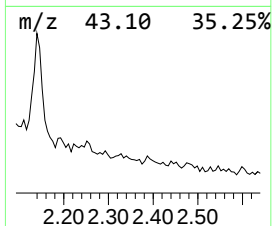
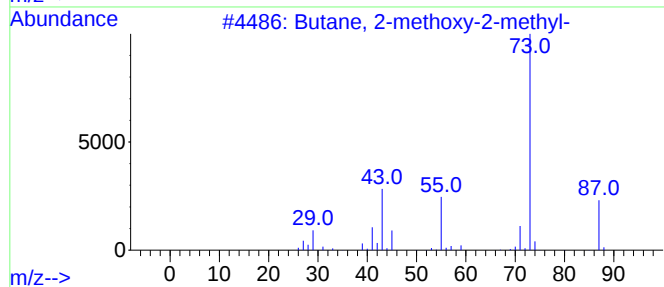
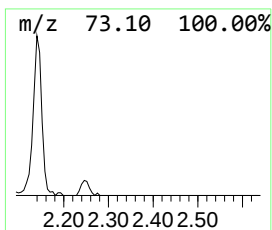
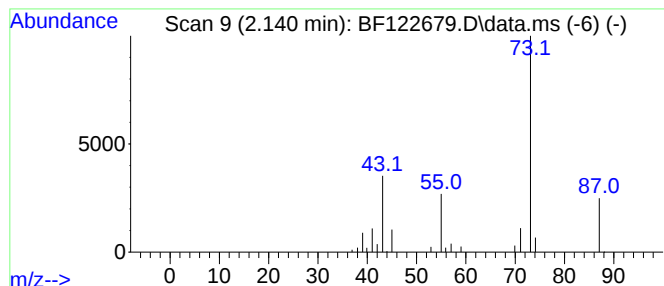
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.140	2.81 ng	115835	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			N-Ethylformamide	73	C3H7NO	000627-45-2	9
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9
5			1,4-Butanediamine	88	C4H12N2	000110-60-1	9



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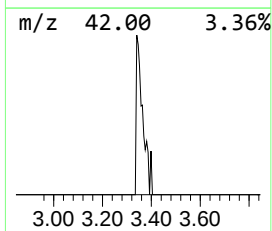
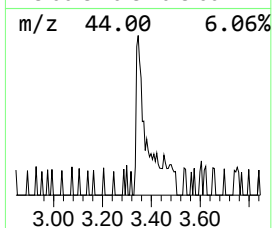
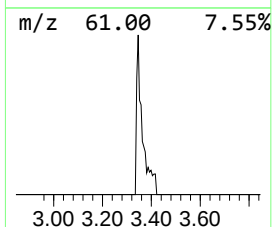
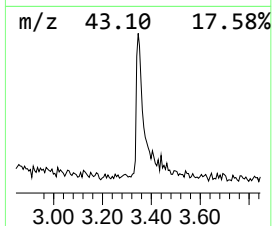
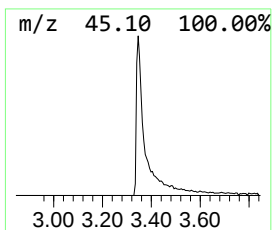
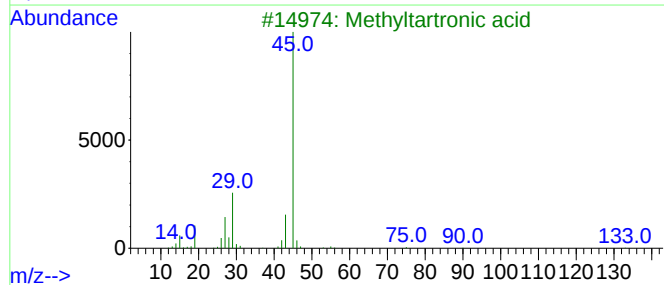
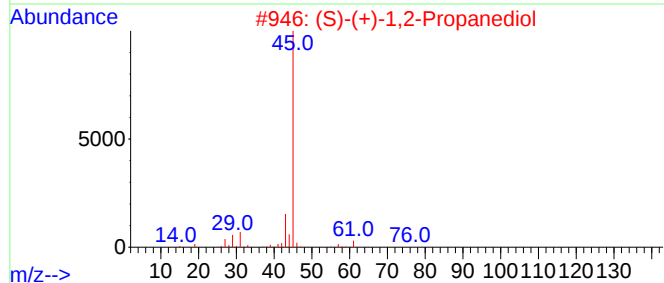
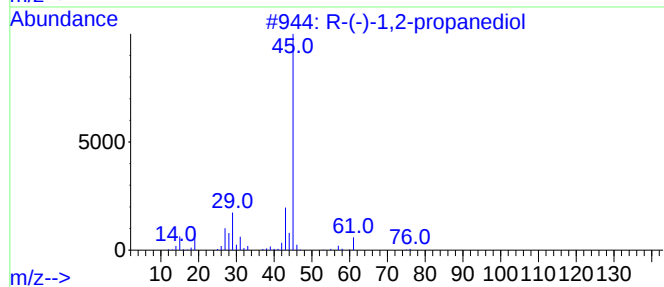
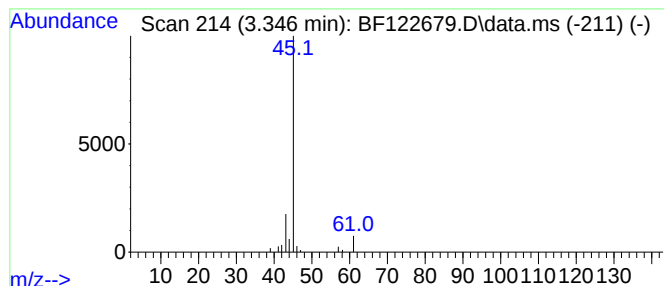
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 R-(-)-1,2-propanediol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.346	2.50 ng	103163	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
2			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
3			Methyltartronic acid	134	C4H6O5	000595-98-2	9
4			Propylene Glycol	76	C3H8O2	000057-55-6	9
5			Isopropyl Alcohol	60	C3H8O	000067-63-0	9



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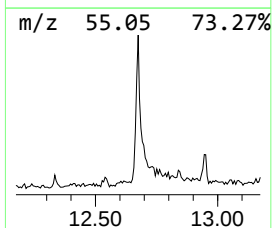
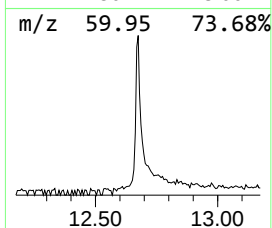
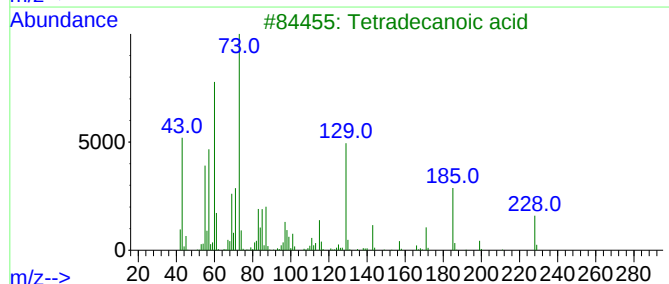
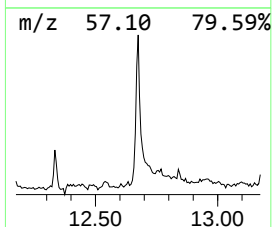
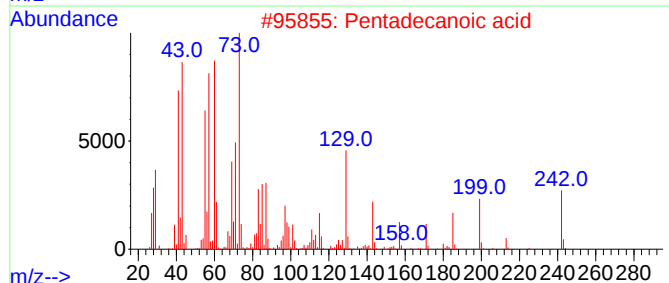
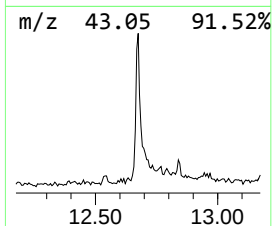
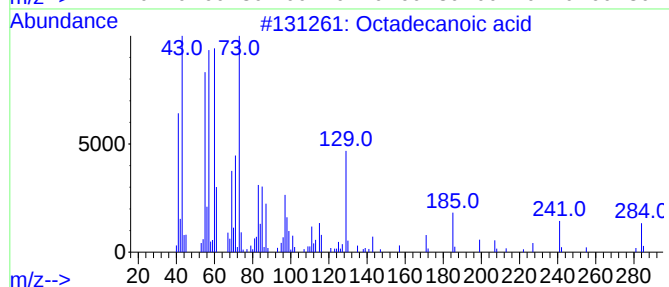
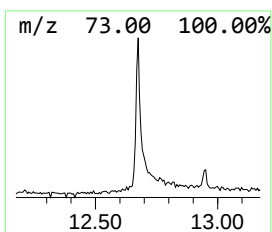
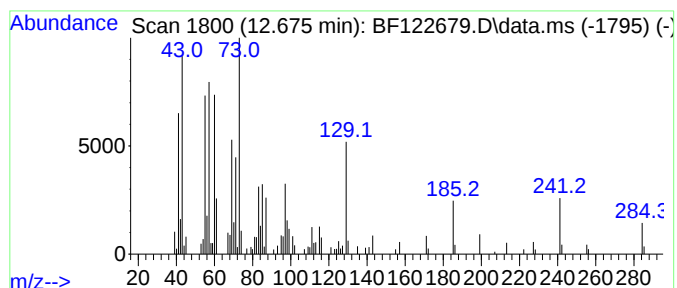
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.675	4.12 ng	269626	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4			n-Decanoic acid	172	C10H20O2	000334-48-5	58
5			Undecanoic acid	186	C11H22O2	000112-37-8	43



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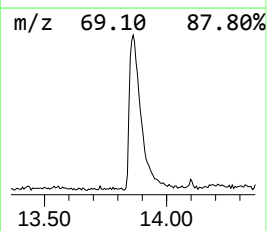
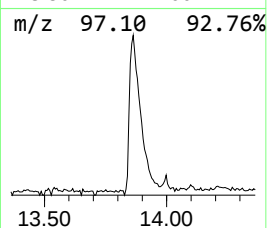
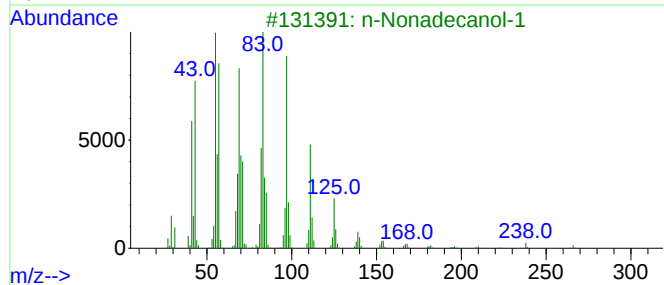
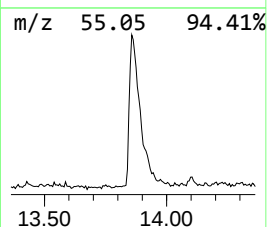
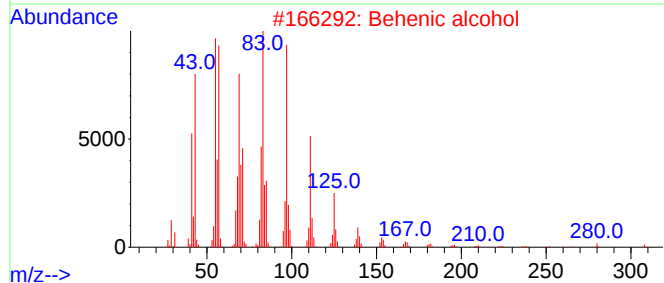
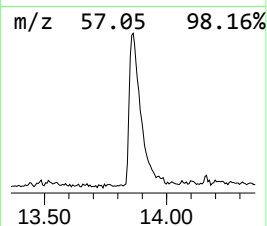
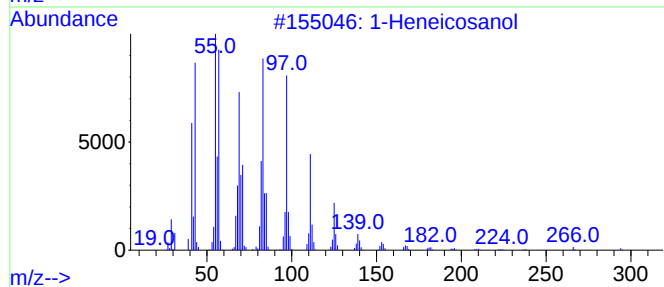
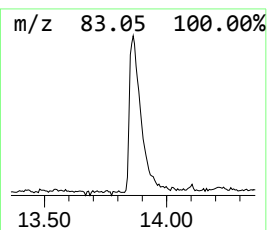
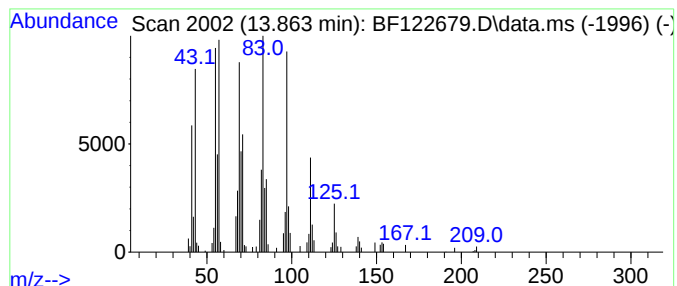
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Peak Number 4 1-Heneicosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	11.67 ng	680112	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			Behenic alcohol	326	C22H46O	000661-19-8	95
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4			1-Heptacosanol	396	C27H56O	002004-39-9	94
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.140	2.8	ng	115835	1	6.834	825400	20.0
R-(-)-1,2-propa...	3.346	2.5	ng	103163	1	6.834	825400	20.0
Octadecanoic acid	12.675	4.1	ng	269626	4	11.357	1307590	20.0
1-Heneicosanol	13.863	11.7	ng	680112	5	13.998	1165930	20.0