

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110922\
 Data File : BF131097.D
 Acq On : 09 Nov 2022 20:34
 Operator : CG\JU
 Sample : N5439-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 506D-3

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-BF110922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131097.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	7	13	19	rVB	1668022	2084274	85.24%	14.656%
2	4.487	405	408	415	rVB	52030	56672	2.32%	0.398%
3	5.098	509	512	518	rBV	149605	157470	6.44%	1.107%
4	5.504	577	581	591	rBV	770077	709286	29.01%	4.987%
5	6.510	748	752	760	rBV	659338	533665	21.83%	3.753%
6	6.886	813	816	820	rBV	615395	549780	22.48%	3.866%
7	7.457	907	913	916	rBV	1328116	1327413	54.29%	9.334%
8	8.175	1030	1035	1038	rBV	850805	707091	28.92%	4.972%
9	9.251	1213	1218	1221	rBV	2893140	2445182	100.00%	17.194%
10	9.933	1329	1334	1337	rBV	1006388	814628	33.32%	5.728%
11	10.722	1464	1468	1472	rBV	1185060	1019974	41.71%	7.172%
12	11.421	1583	1587	1591	rBV	946152	839868	34.35%	5.906%
13	13.010	1853	1857	1861	rBV	1997995	1695076	69.32%	11.919%
14	13.986	2016	2023	2030	rBV4	38194	119541	4.89%	0.841%
15	14.068	2034	2037	2041	rVB	705786	595861	24.37%	4.190%
16	14.162	2048	2053	2058	rBV	61918	58094	2.38%	0.408%
17	14.915	2178	2181	2185	rBV	29976	31607	1.29%	0.222%
18	15.562	2286	2291	2301	rVB	386918	475880	19.46%	3.346%

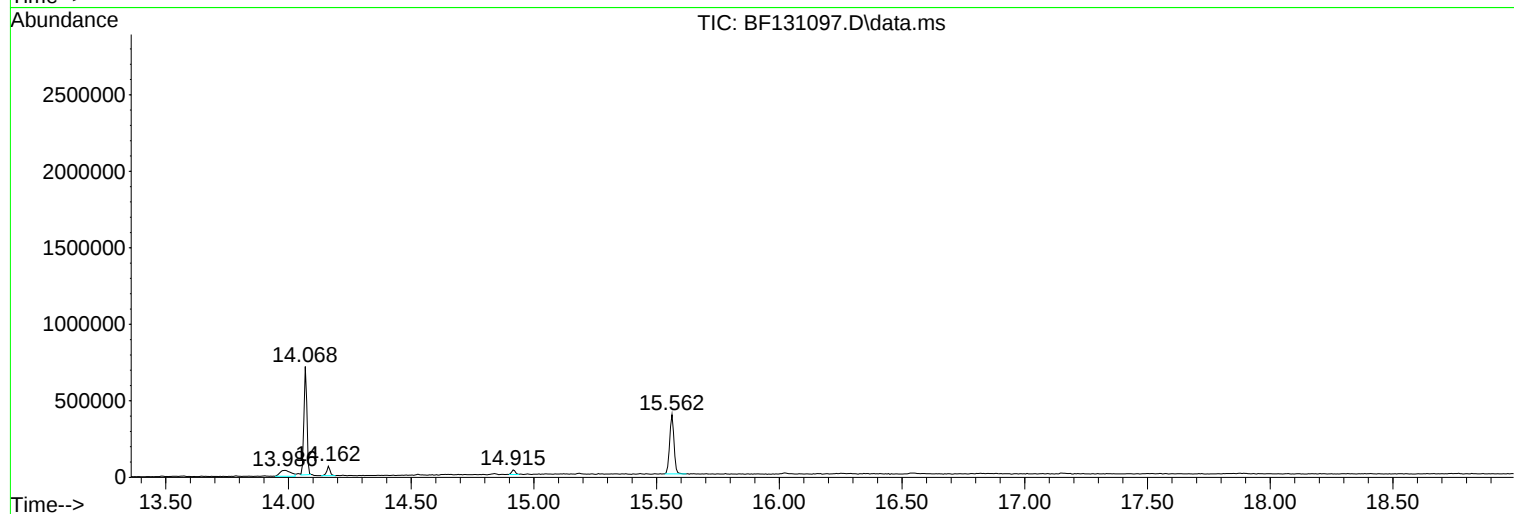
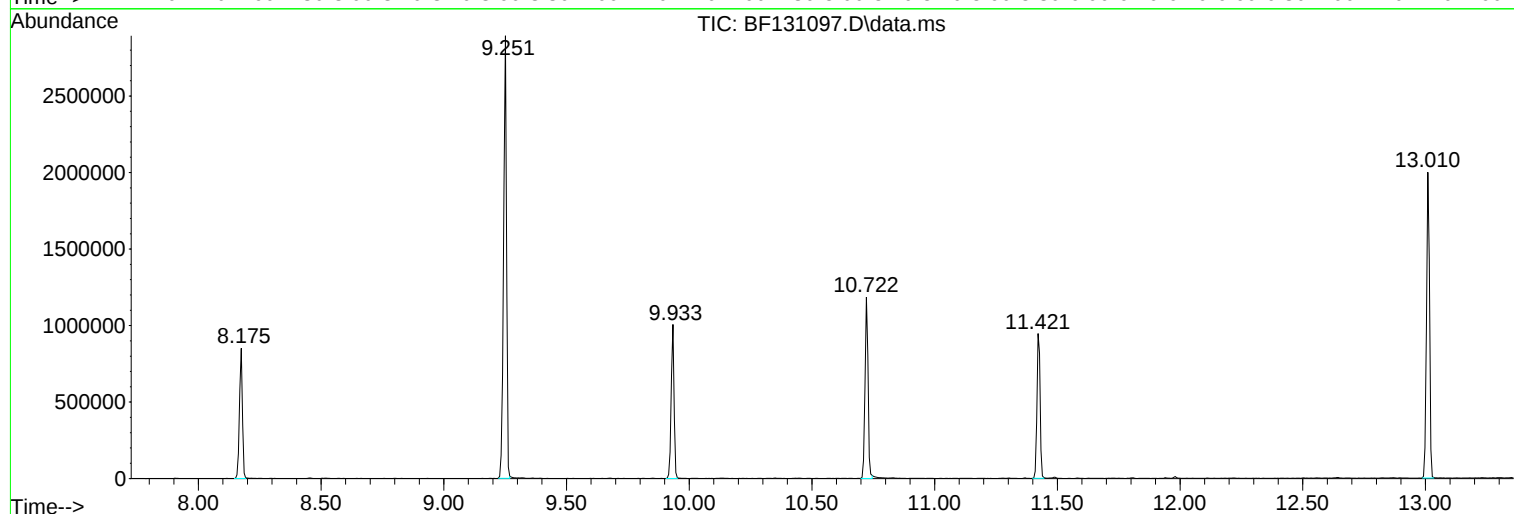
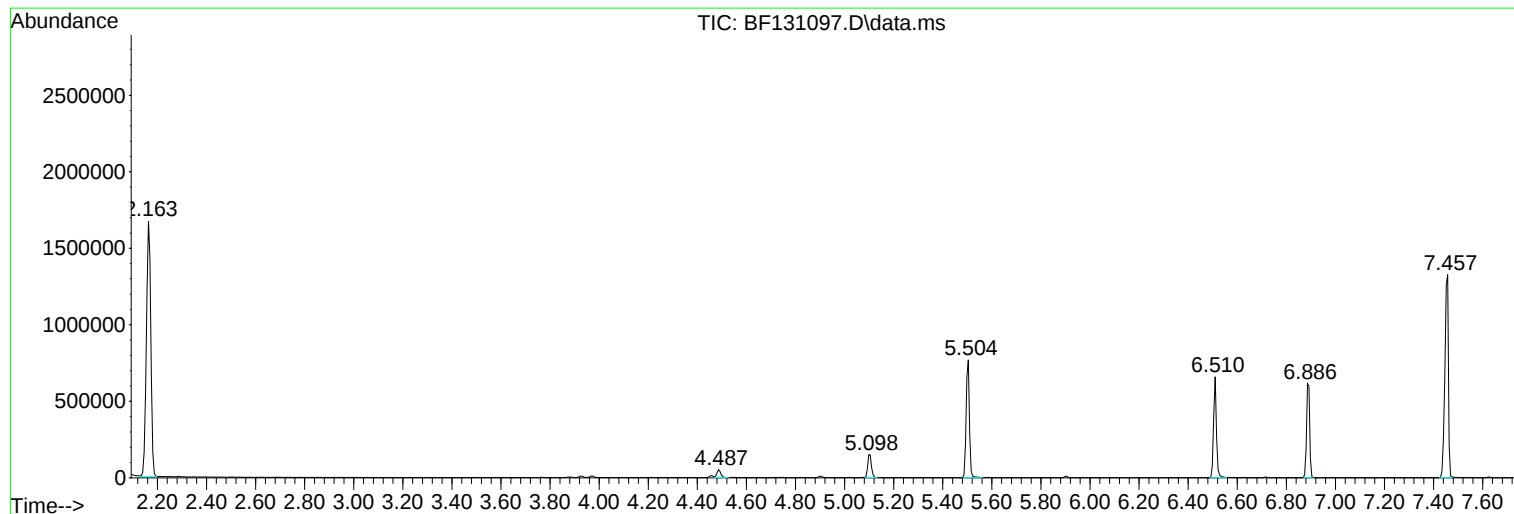
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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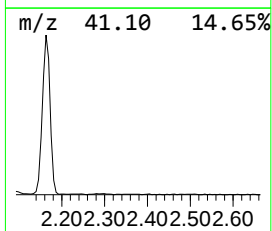
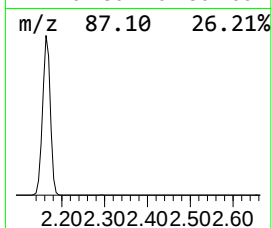
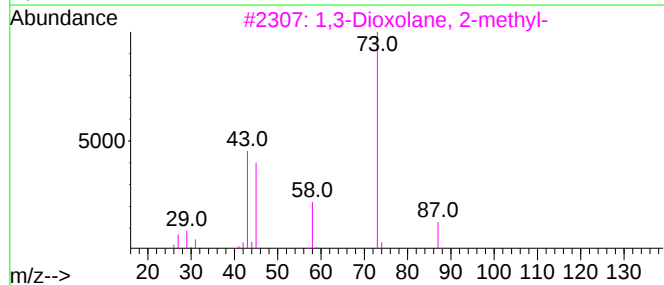
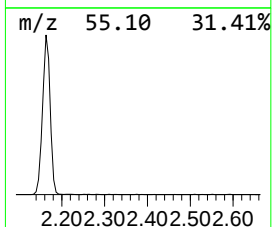
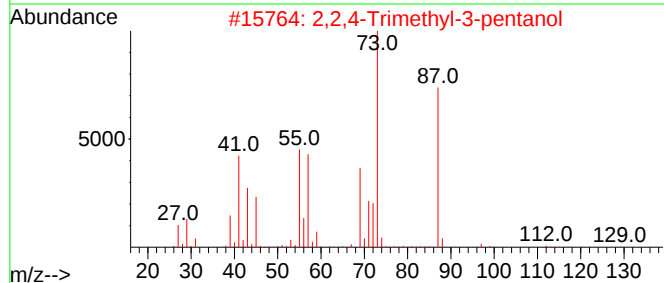
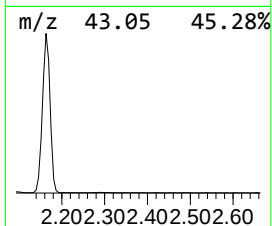
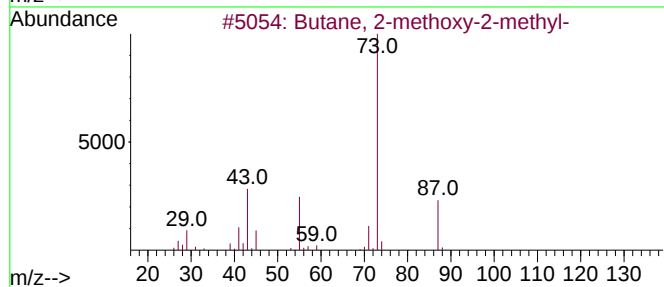
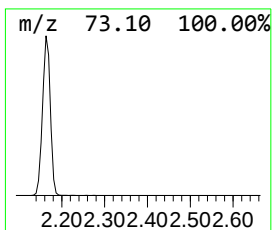
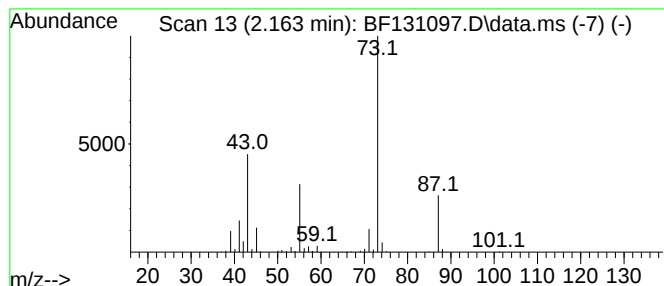
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.163	75.82 ng	2084270	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	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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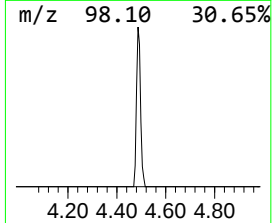
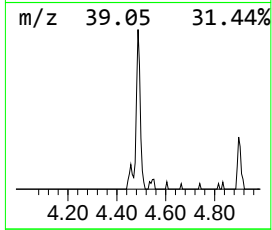
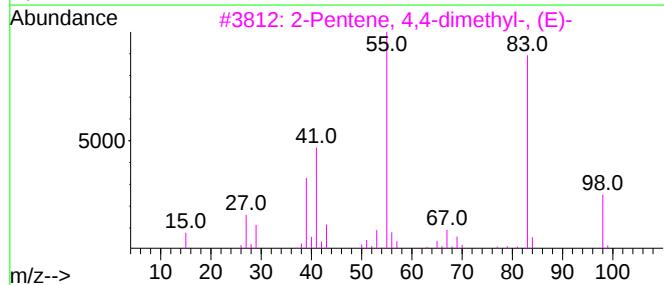
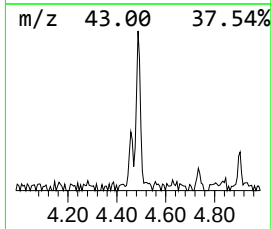
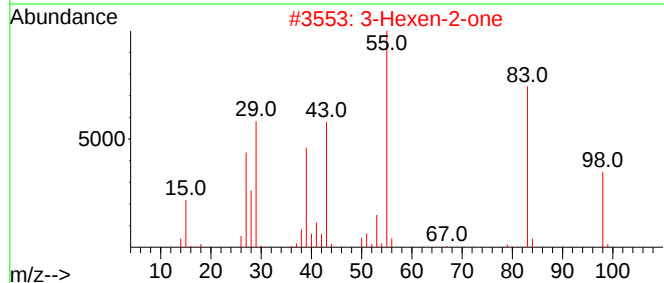
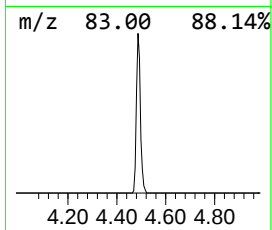
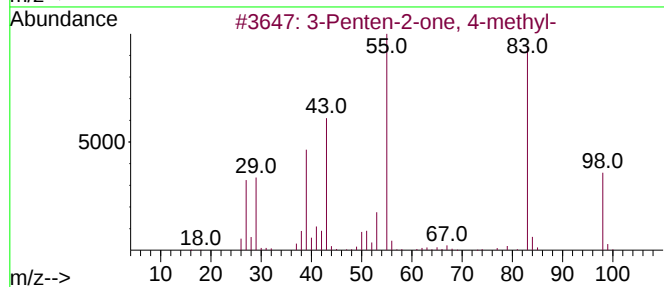
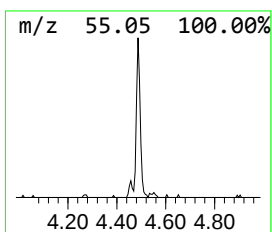
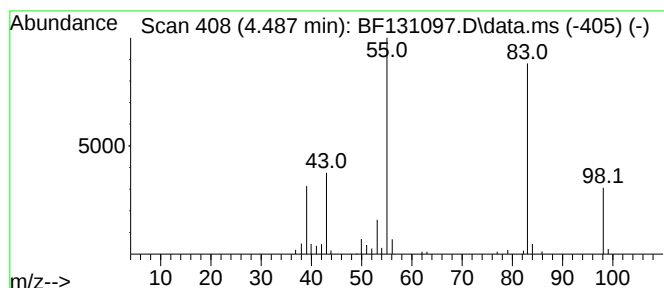
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.487	2.06 ng	56672	1,4-Dichlorobenzene-d4	6.892

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	90
3		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	90
4		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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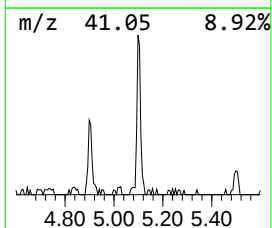
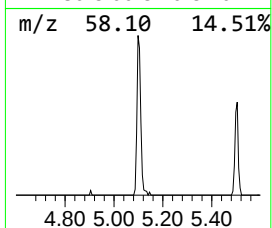
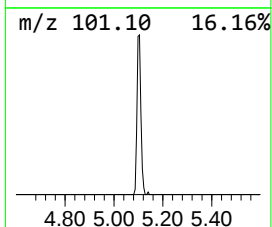
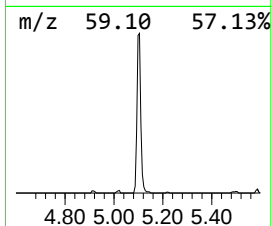
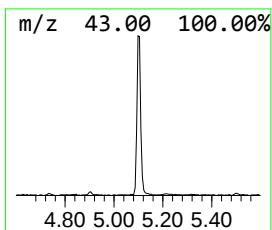
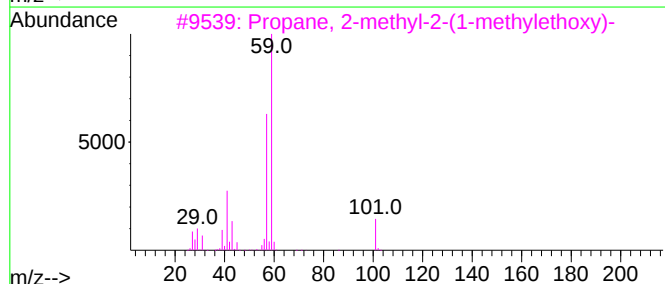
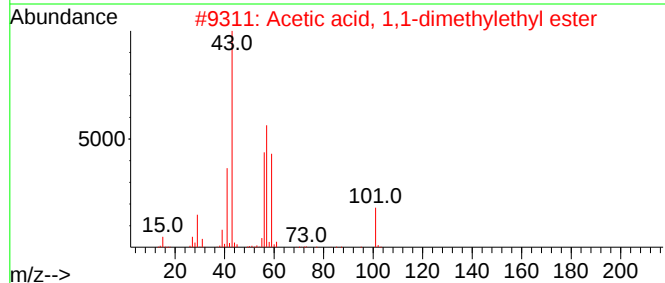
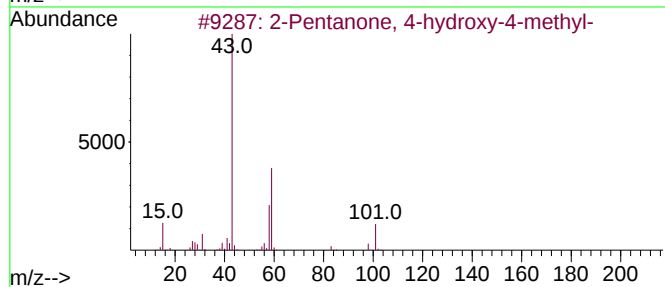
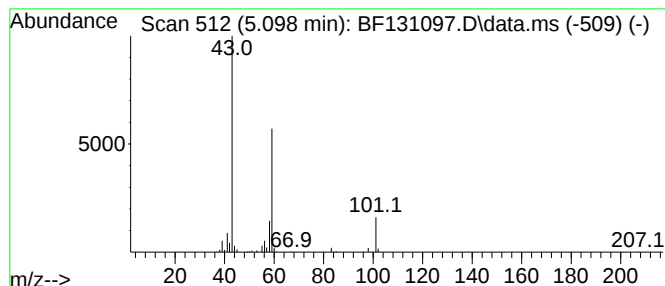
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	5.73 ng	157470	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	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			3-Hexanol	102	C6H14O	000623-37-0	33



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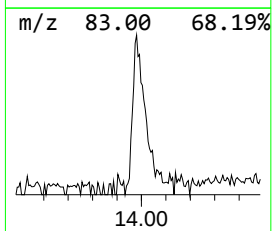
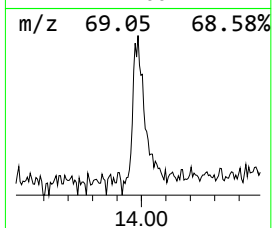
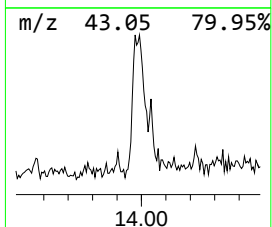
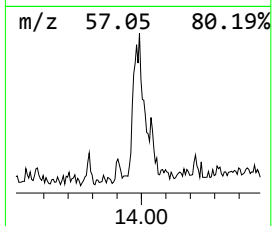
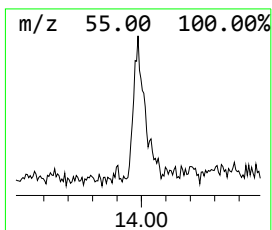
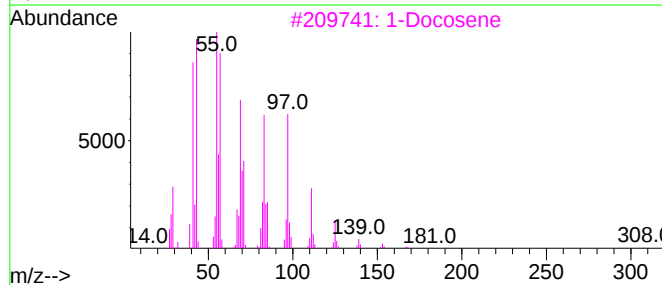
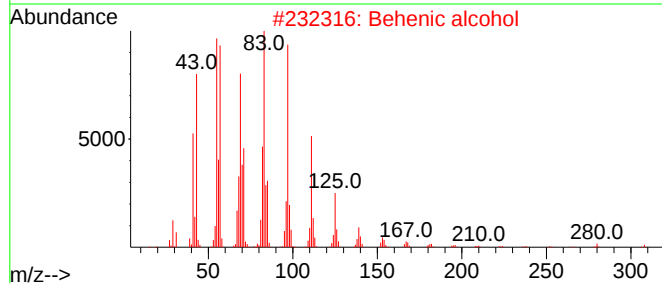
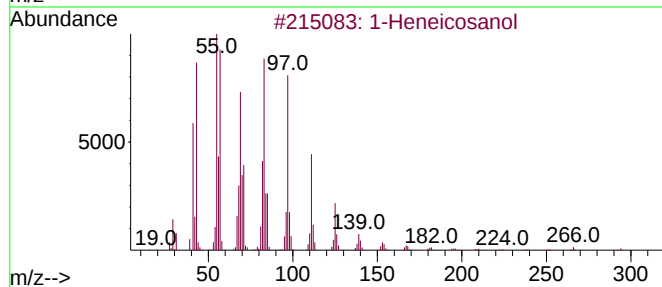
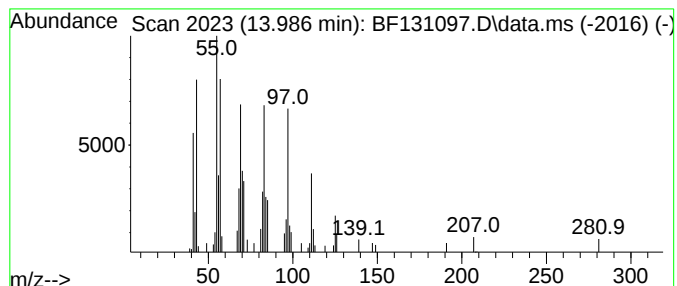
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Peak Number 4 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.986	4.01 ng	119541	Chrysene-d12	14.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	93
2			Behenic alcohol	326	C22H46O	000661-19-8	93
3			1-Docosene	308	C22H44	001599-67-3	91
4			1-Tricosene	322	C23H46	018835-32-0	91
5			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.163	75.8	ng	2084270	1	6.892	549780	20.0
3-Penten-2-one,...	4.487	2.1	ng	56672	1	6.892	549780	20.0
2-Pentanone, 4-...	5.098	5.7	ng	157470	1	6.892	549780	20.0
1-Heneicosanol	13.986	4.0	ng	119541	5	14.068	595861	20.0