

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080222\
 Data File : BF129520.D
 Acq On : 02 Aug 2022 22:09
 Operator : CG\JU
 Sample : N3996-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MH-CS

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-BF072522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129520.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.481	369	373	381	rBV	213580	241099	5.08%	0.868%
2	5.110	477	480	489	rVB	128175	159838	3.37%	0.575%
3	5.516	544	549	552	rBV	4349329	4128116	86.95%	14.861%
4	6.522	715	720	723	rBV	4042272	4191338	88.28%	15.088%
5	6.875	776	780	783	rBV	1173778	890398	18.75%	3.205%
6	7.439	871	876	879	rBV	2885409	2776212	58.48%	9.994%
7	8.157	994	998	1001	rBV	1532852	1160913	24.45%	4.179%
8	9.233	1176	1181	1184	rBV	5902429	4747609	100.00%	17.091%
9	9.916	1293	1297	1300	rBV	1419611	1178844	24.83%	4.244%
10	10.710	1427	1432	1435	rBV	2381888	2248002	47.35%	8.093%
11	11.404	1546	1550	1553	rBV	1093367	942757	19.86%	3.394%
12	11.916	1632	1637	1642	rBV2	65228	93496	1.97%	0.337%
13	12.345	1706	1710	1713	rBV	69399	56423	1.19%	0.203%
14	12.615	1753	1756	1761	rBV	71275	75934	1.60%	0.273%
15	12.845	1790	1795	1798	rBV	69150	81164	1.71%	0.292%
16	12.986	1815	1819	1823	rBV	3395179	3147734	66.30%	11.331%
17	13.880	1967	1971	1979	rBV3	89226	150313	3.17%	0.541%
18	14.045	1995	1999	2002	rBV	871155	798872	16.83%	2.876%
19	14.792	2123	2126	2131	rBV2	72867	84662	1.78%	0.305%
20	15.533	2248	2252	2257	rVB2	501804	624965	13.16%	2.250%

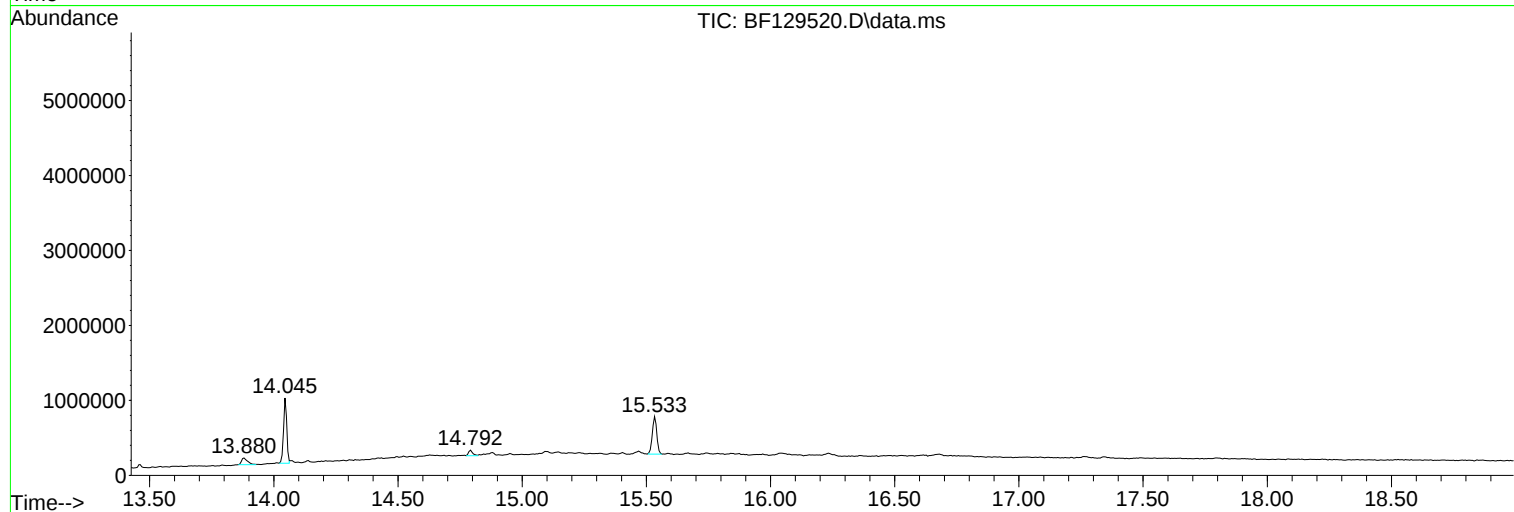
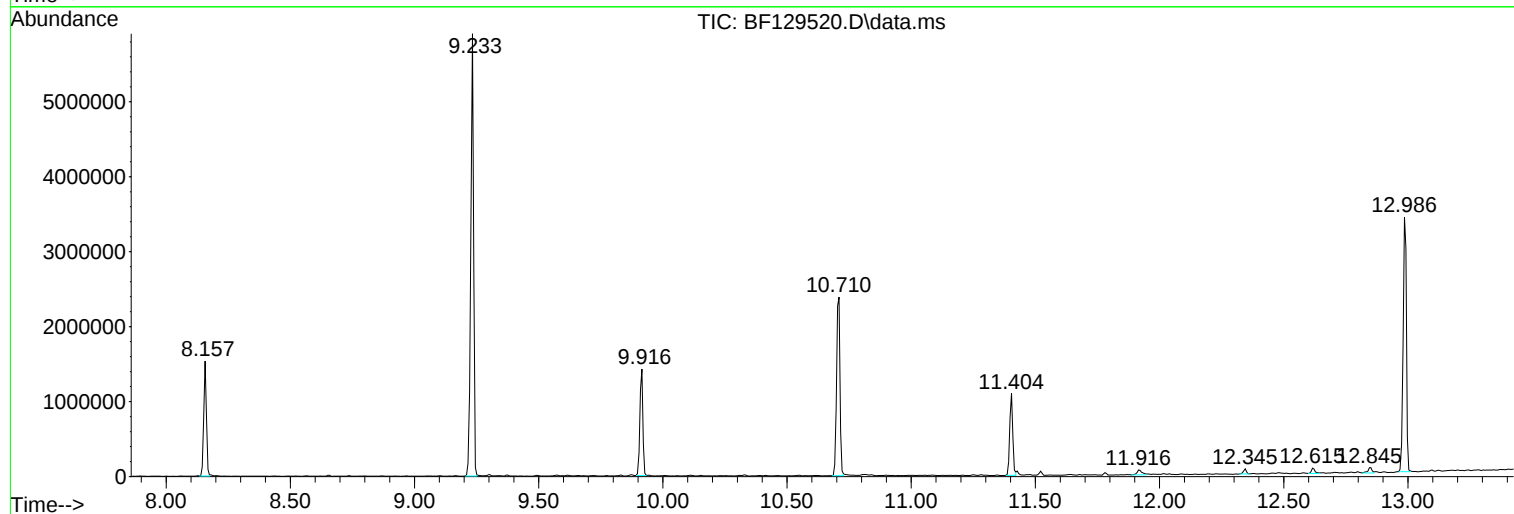
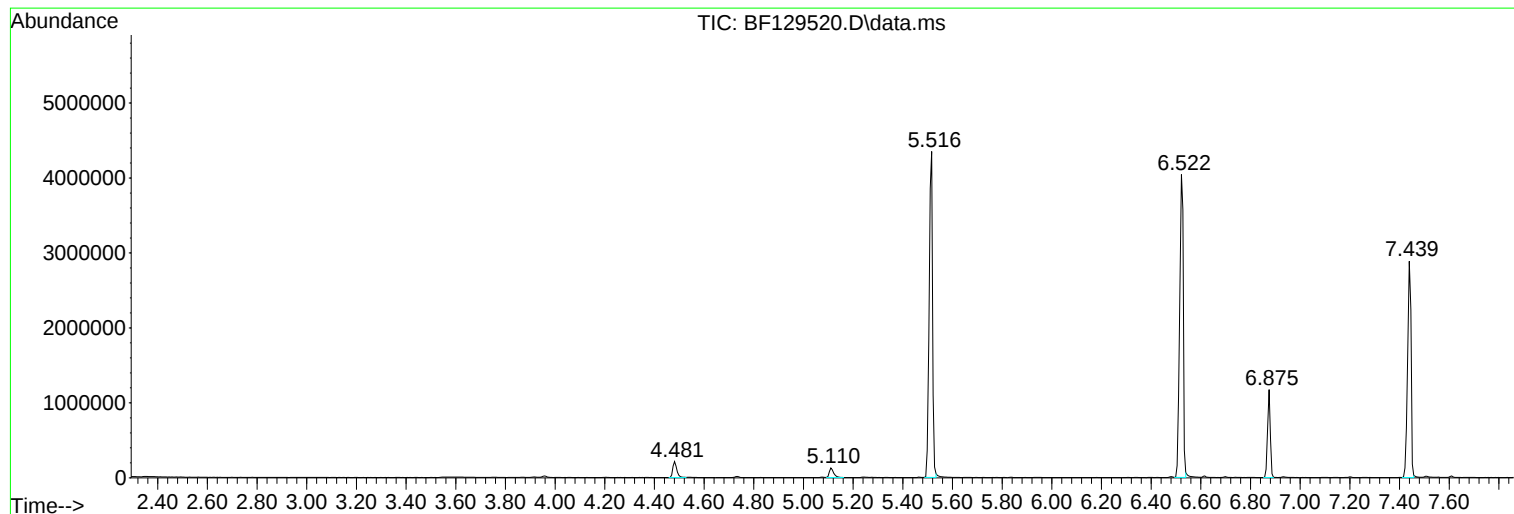
Sum of corrected areas: 27778689

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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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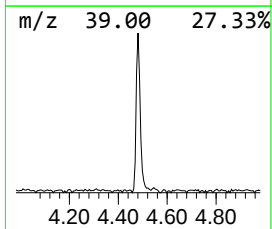
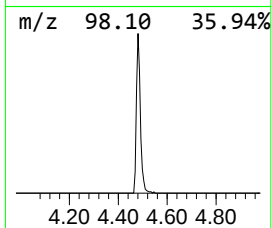
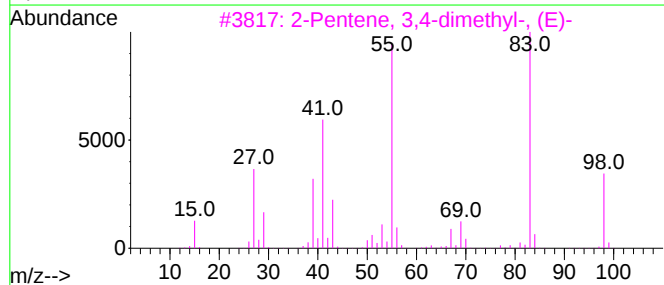
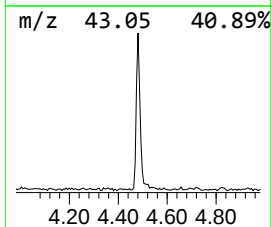
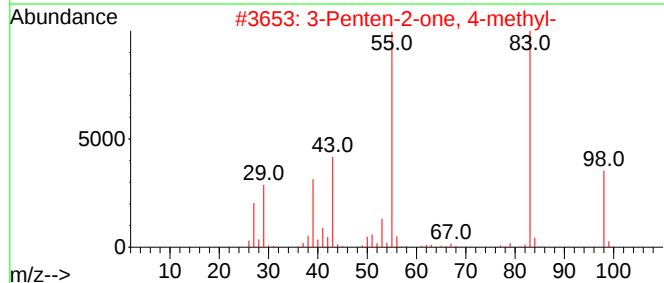
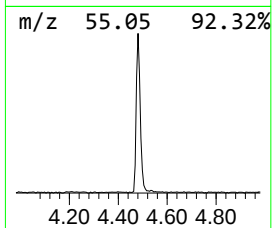
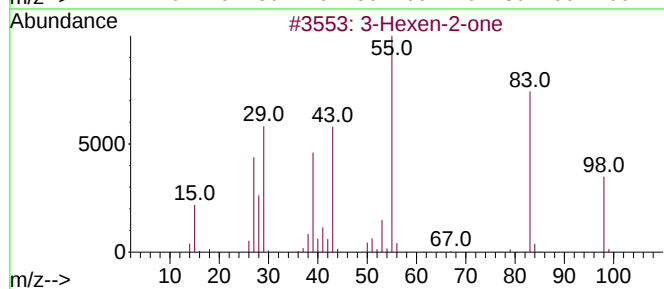
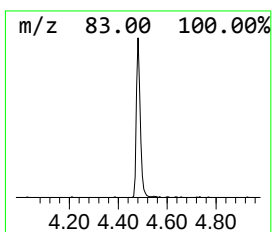
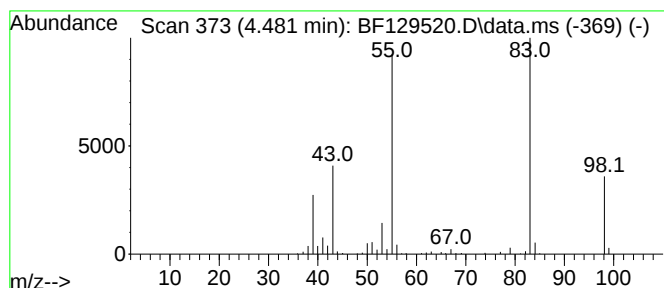
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Hexen-2-one Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.481	5.42 ng	241099	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	91
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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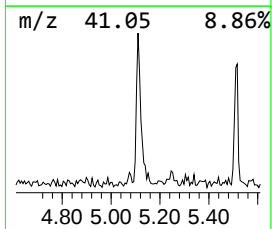
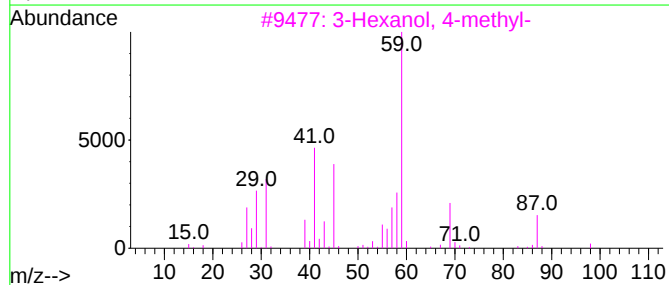
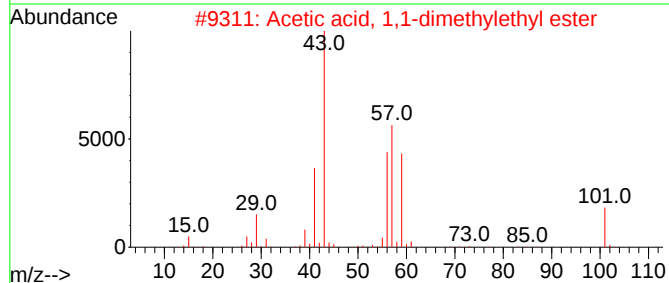
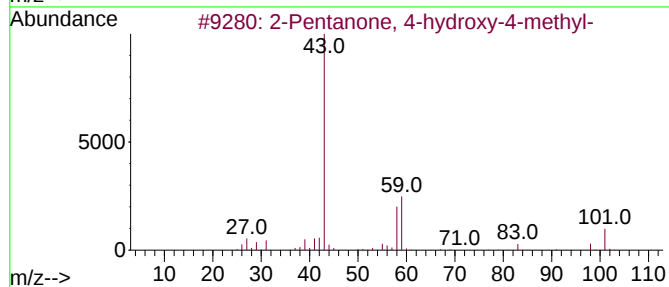
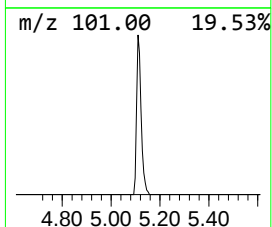
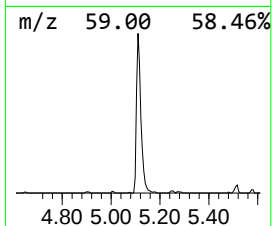
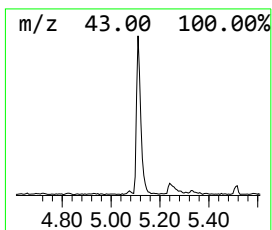
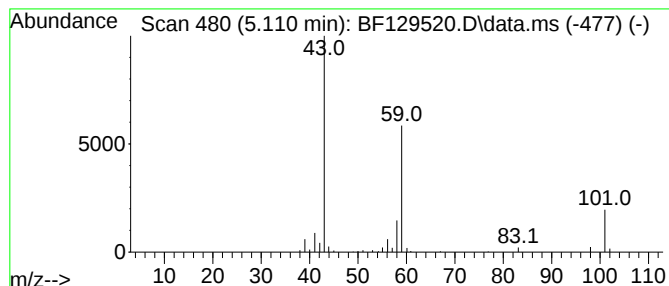
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	3.59 ng	159838	1,4-Dichlorobenzene-d4	6.875

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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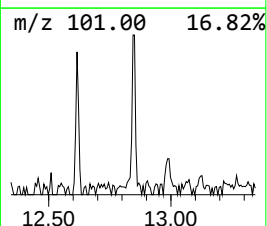
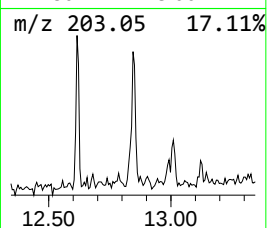
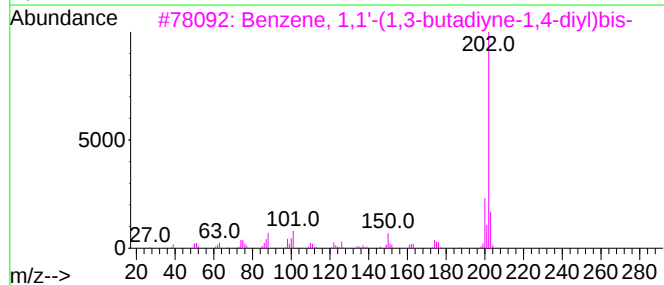
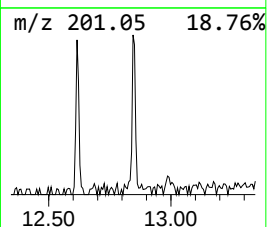
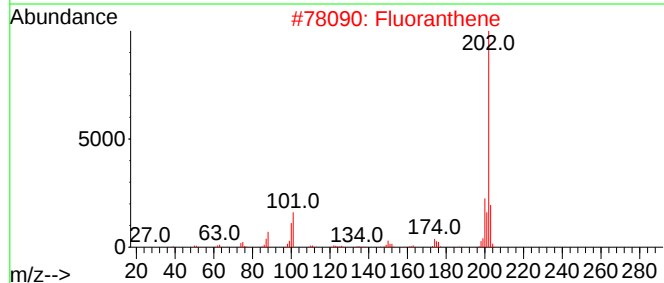
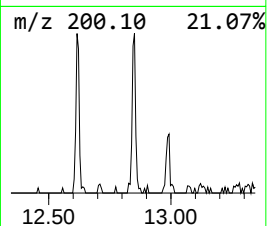
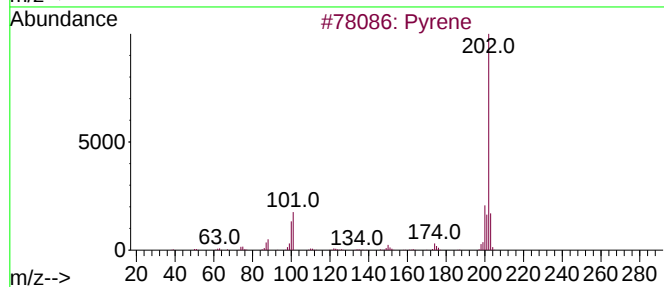
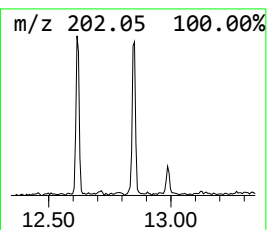
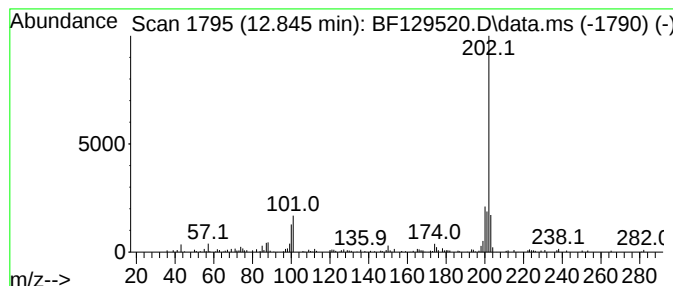
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.845	2.03 ng	81164	Chrysene-d12	14.045	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene	202	C16H10	000129-00-0	94
2	Fluoranthene	202	C16H10	000206-44-0	90
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	59
4	4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	52
5	l-Leucine, N-methyl-N-(2-methoxy...	485	C28H55NO5	1010328-55-1	47



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Instrument :
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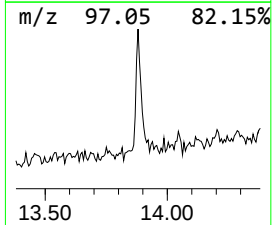
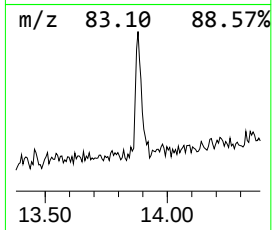
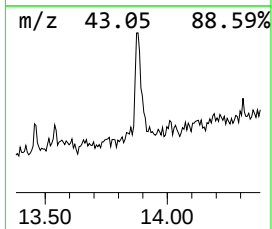
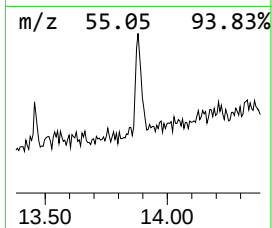
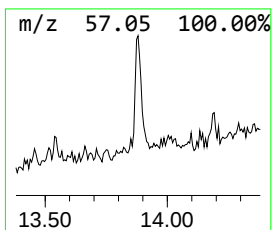
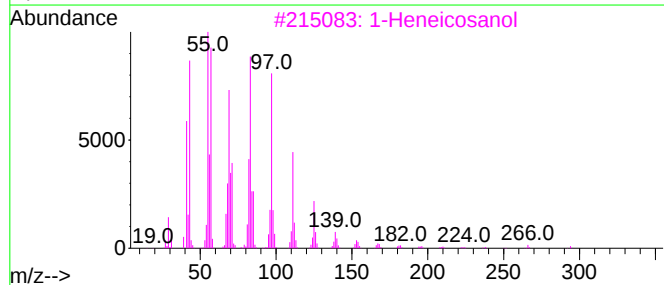
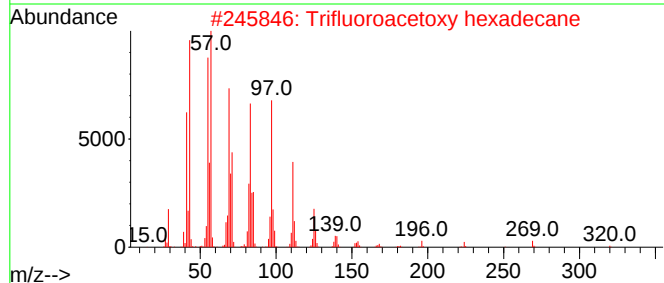
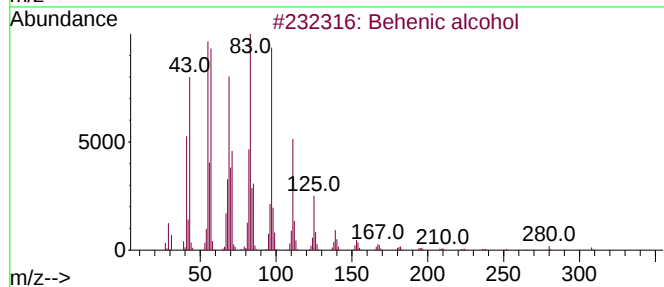
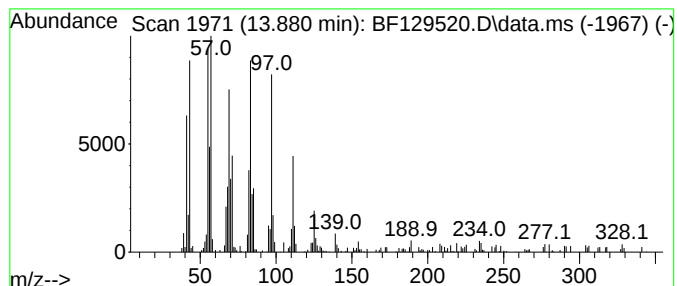
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Peak Number 4 Behenic alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	3.76 ng	150313	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	94
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3			1-Heneicosanol	312	C21H44O	015594-90-8	94
4			1-Heptacosanol	396	C27H56O	002004-39-9	94
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94



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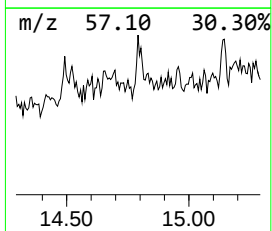
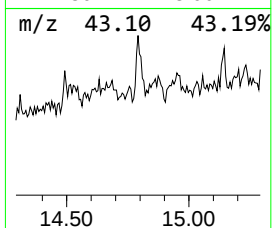
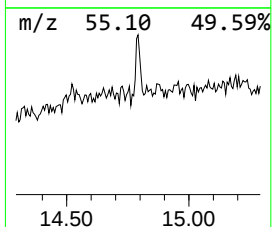
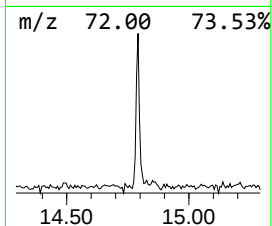
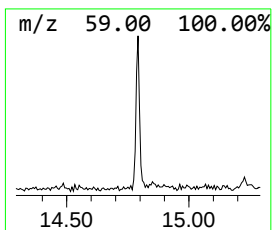
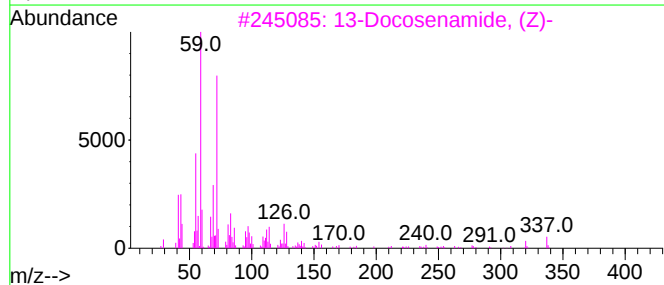
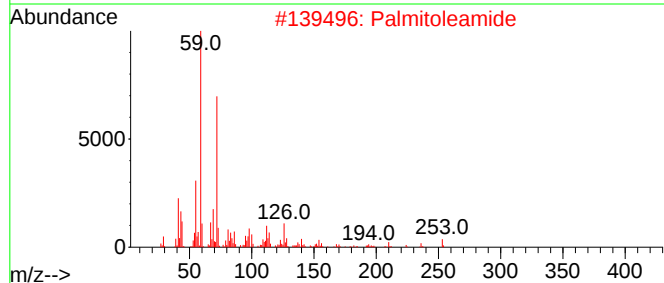
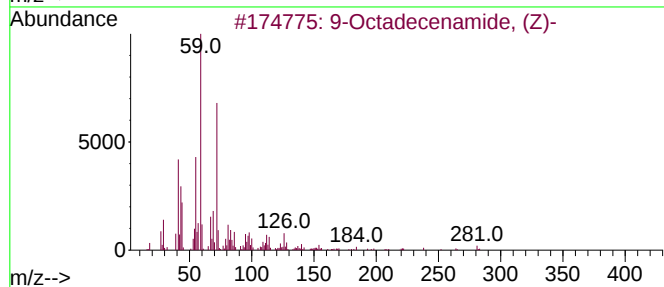
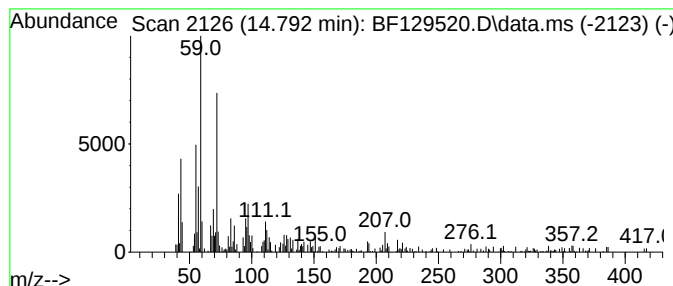
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.792	2.71 ng	84662	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	78
2			Palmitoleamide	253	C16H31NO	106010-22-4	64
3			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	64
4			Hexadecanamide	255	C16H33NO	000629-54-9	59
5			Dodecanamide	199	C12H25NO	001120-16-7	41



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Hexen-2-one	4.481	5.4	ng	241099	1	6.875	890398	20.0
2-Pentanone, 4-...	5.110	3.6	ng	159838	1	6.875	890398	20.0
Benzene, 1,1'-(...	12.845	2.0	ng	81164	5	14.045	798872	20.0
Behenic alcohol	13.880	3.8	ng	150313	5	14.045	798872	20.0
9-Octadecenamid...	14.792	2.7	ng	84662	6	15.533	624965	20.0