

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101923\
 Data File : BF135889.D
 Acq On : 19 Oct 2023 16:38
 Operator : CG\JU
 Sample : 04908-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-1

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-BF101323.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135889.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.957	484	488	503	rBV	482821	622479	40.25%	5.362%
2	5.375	556	559	584	rBV	1392795	1546602	100.00%	13.321%
3	6.393	729	732	748	rBV	1243215	1250135	80.83%	10.768%
4	6.734	787	790	799	rVB	449930	380468	24.60%	3.277%
5	7.304	884	887	905	rBV	951258	833891	53.92%	7.183%
6	8.016	1004	1008	1025	rVB	468708	424313	27.44%	3.655%
7	9.092	1187	1191	1194	rBV	1888360	1485016	96.02%	12.791%
8	9.210	1207	1211	1216	rVB	23756	21802	1.41%	0.188%
9	9.769	1303	1306	1314	rBV	601930	549587	35.54%	4.734%
10	10.569	1439	1442	1454	rBV	1096599	1027264	66.42%	8.848%
11	10.939	1503	1505	1511	rBV3	15535	20753	1.34%	0.179%
12	11.269	1558	1561	1569	rBV	578879	494280	31.96%	4.257%
13	11.727	1637	1639	1646	rBV4	20388	30224	1.95%	0.260%
14	11.804	1649	1652	1666	rVV	339165	359712	23.26%	3.098%
15	12.516	1767	1773	1780	rBV5	15606	41520	2.68%	0.358%
16	12.592	1783	1786	1795	rBV2	43725	70574	4.56%	0.608%
17	12.863	1828	1832	1836	rBV	1427853	1295147	83.74%	11.156%
18	13.433	1926	1929	1932	rBV3	18141	18430	1.19%	0.159%
19	13.810	1988	1993	2006	rBV6	30356	95424	6.17%	0.822%
20	13.933	2011	2014	2022	rVB	329211	339452	21.95%	2.924%
21	14.086	2036	2040	2043	rVB	22132	21437	1.39%	0.185%
22	14.392	2089	2092	2097	rBV2	20540	19832	1.28%	0.171%
23	14.698	2141	2144	2148	rVB	19861	21563	1.39%	0.186%
24	14.768	2152	2156	2161	rVB	284871	281936	18.23%	2.428%
25	15.027	2198	2200	2205	rVB2	21952	24427	1.58%	0.210%
26	15.410	2261	2265	2272	rBV	233804	314260	20.32%	2.707%
27	15.839	2336	2338	2342	rVB3	18043	19312	1.25%	0.166%

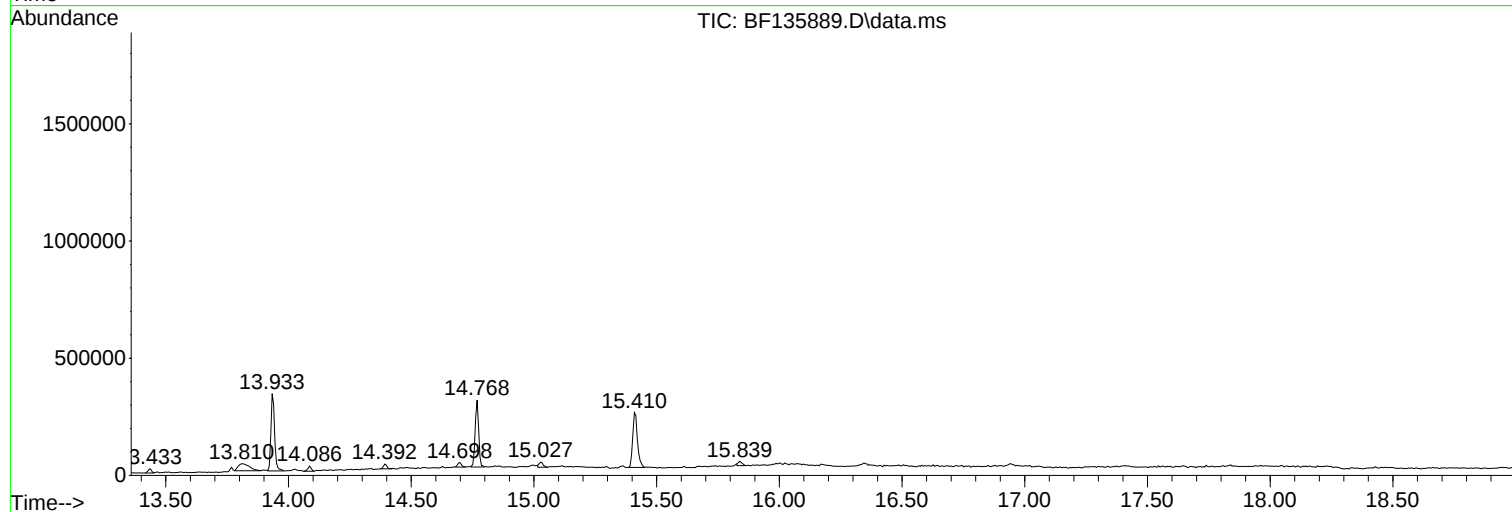
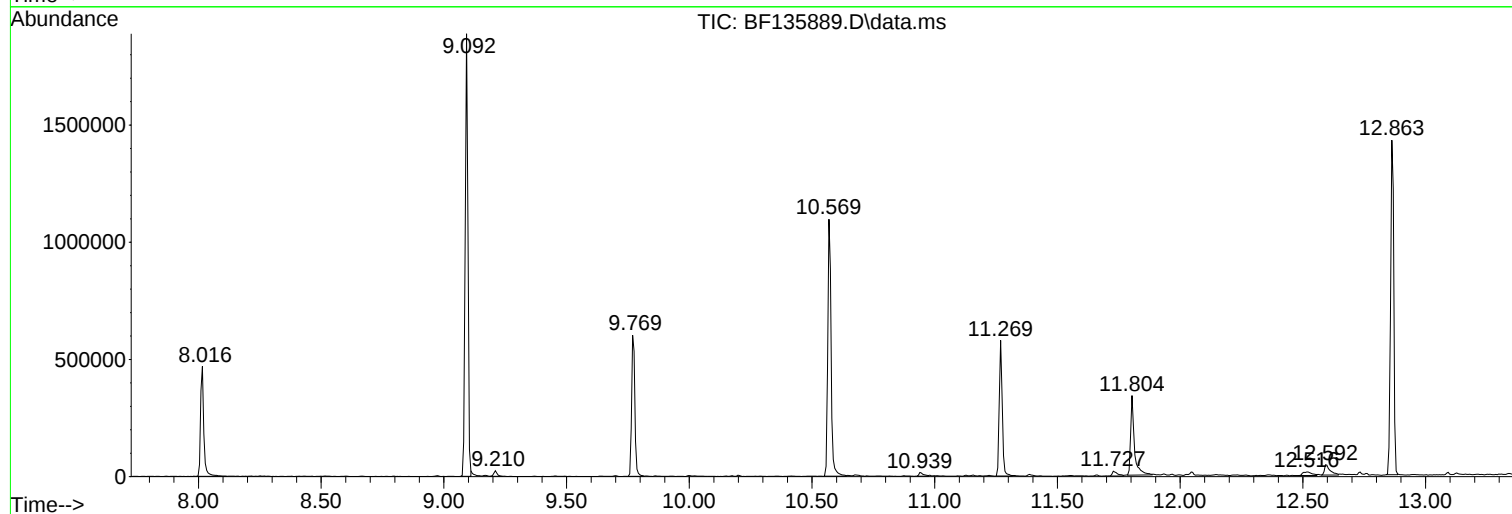
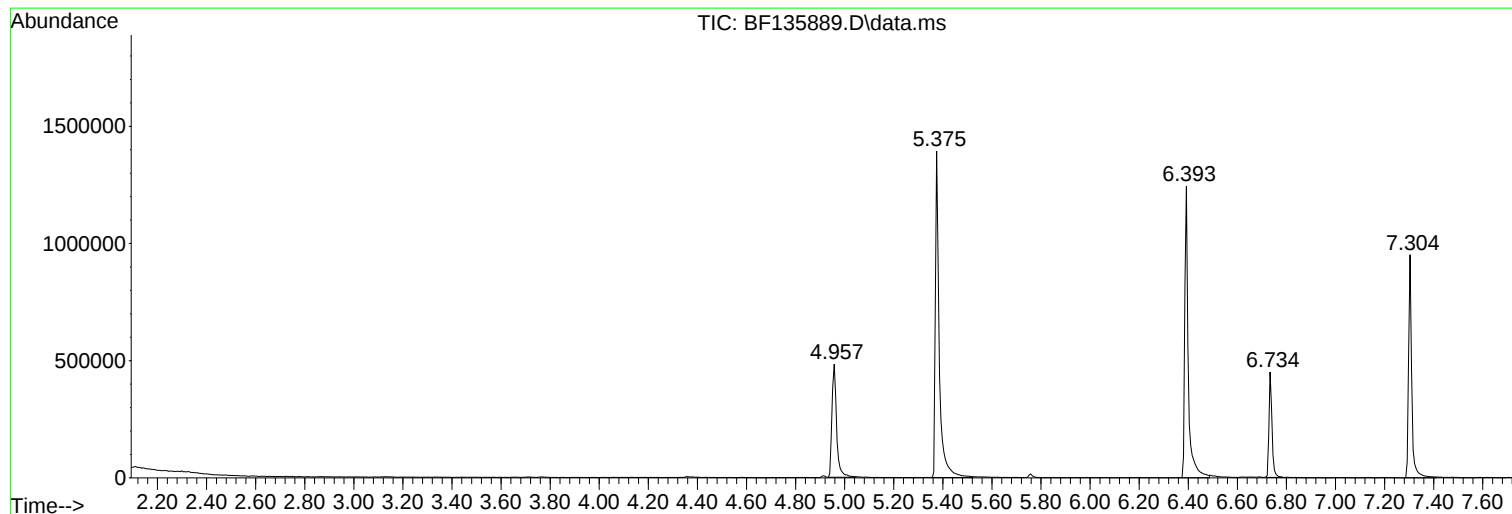
Sum of corrected areas: 11609840

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.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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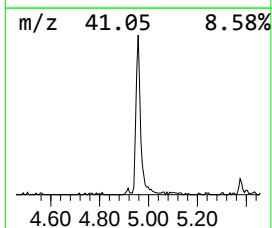
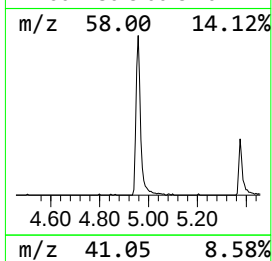
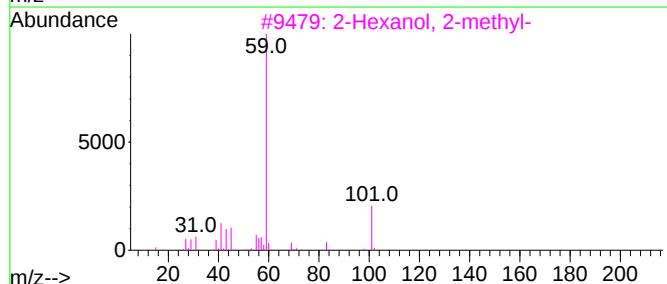
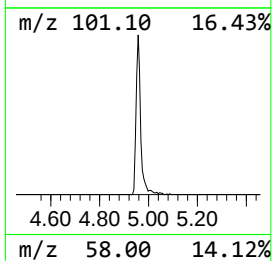
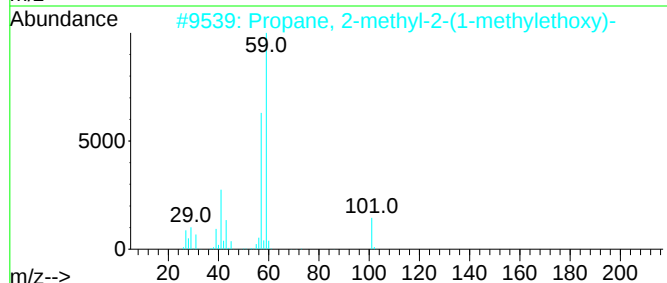
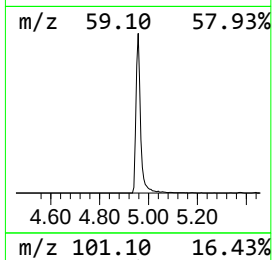
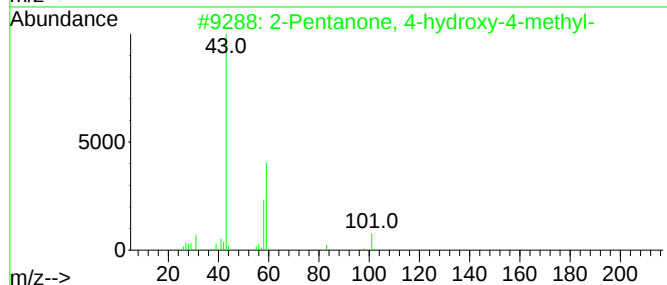
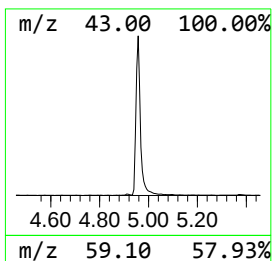
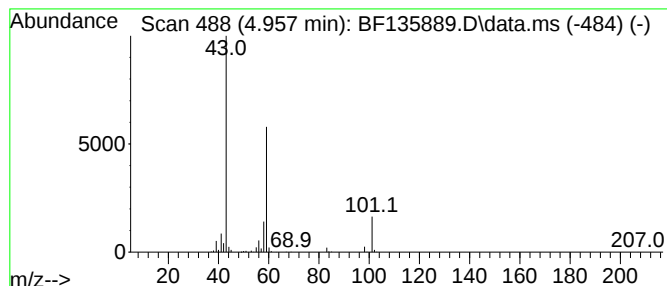
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.957	32.72 ng	622479	1,4-Dichlorobenzene-d4	6.734

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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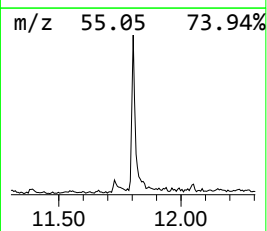
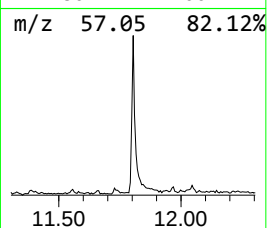
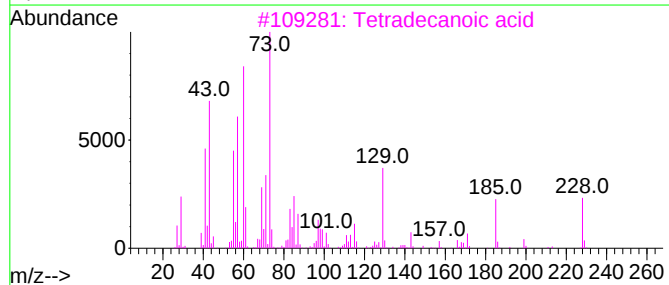
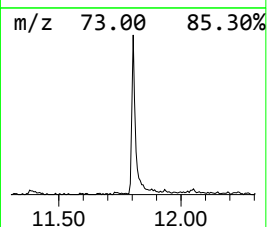
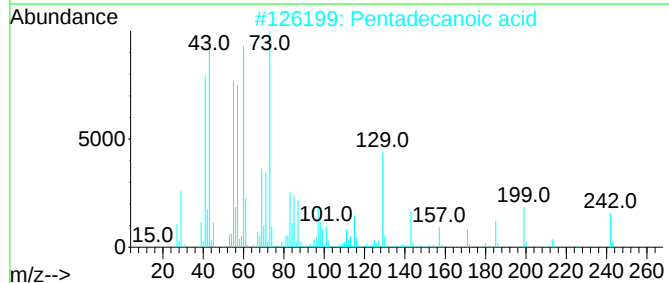
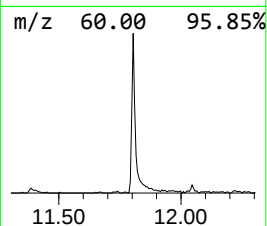
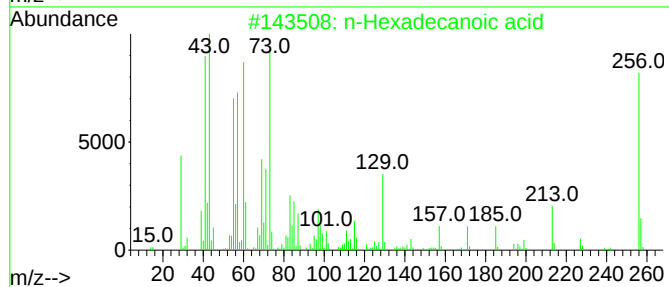
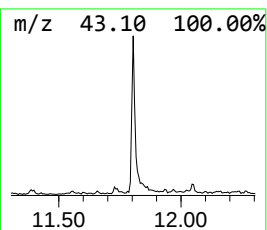
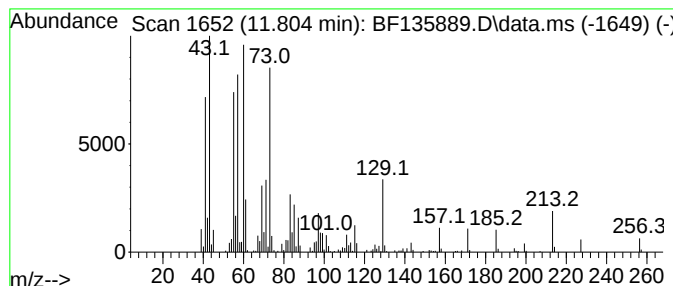
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	14.56 ng	359712	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			Tridecanoic acid	214	C13H26O2	000638-53-9	72
5			Nonanoic acid	158	C9H18O2	000112-05-0	49



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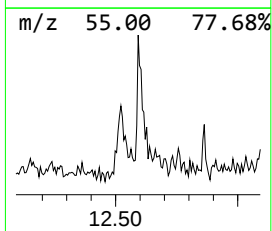
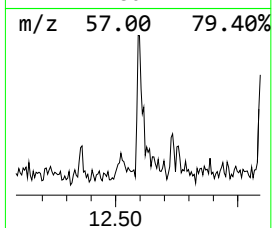
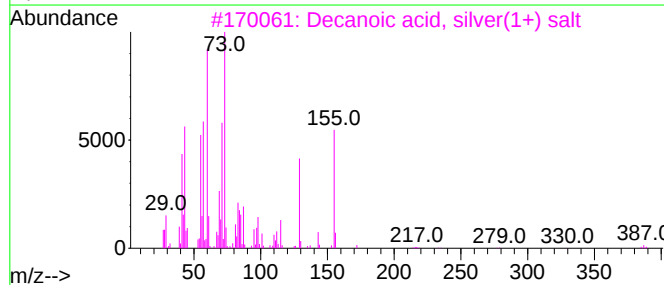
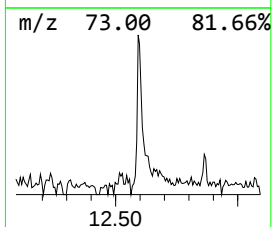
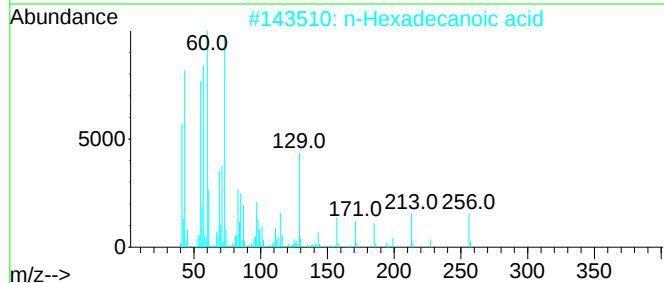
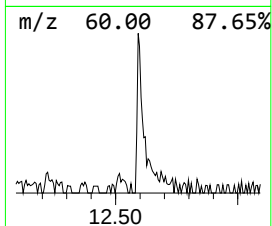
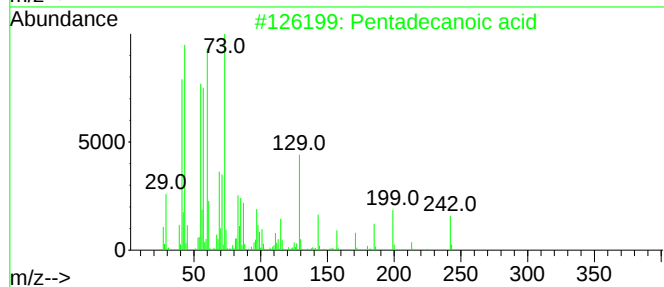
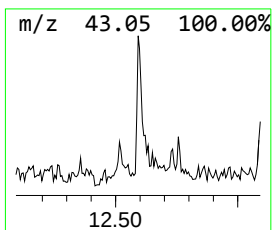
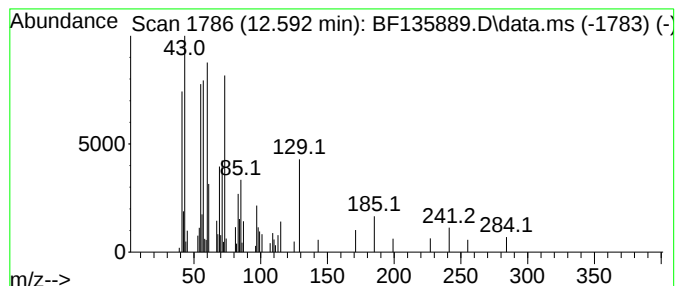
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Pentadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.592	2.86 ng	70574	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
3			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64
4			Octadecanoic acid	284	C18H36O2	000057-11-4	60
5			n-Decanoic acid	172	C10H20O2	000334-48-5	50



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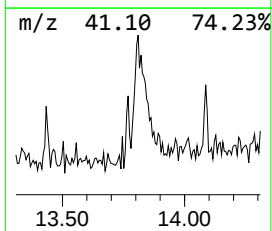
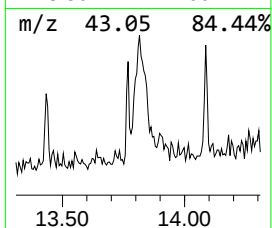
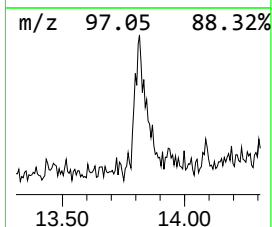
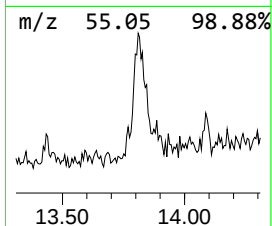
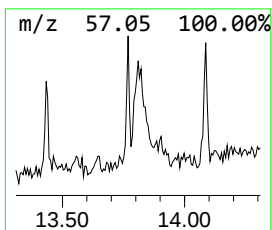
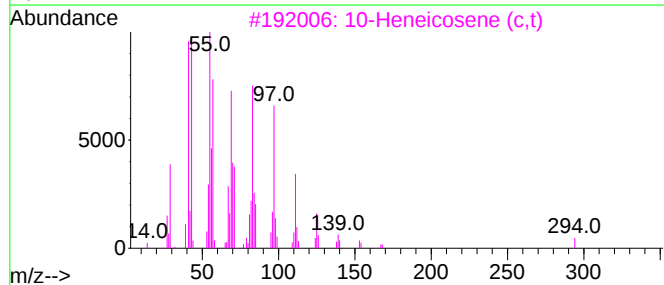
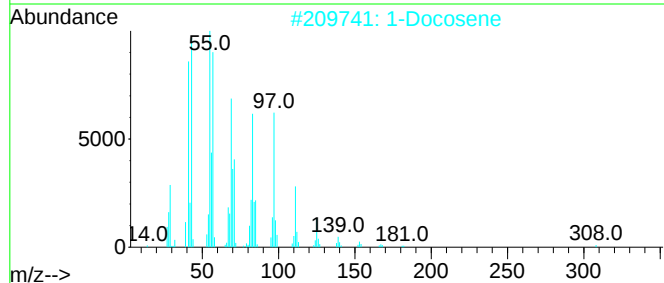
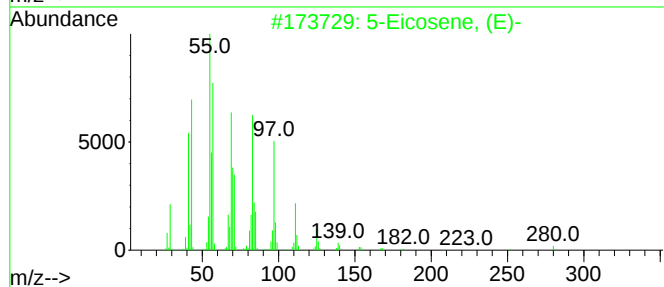
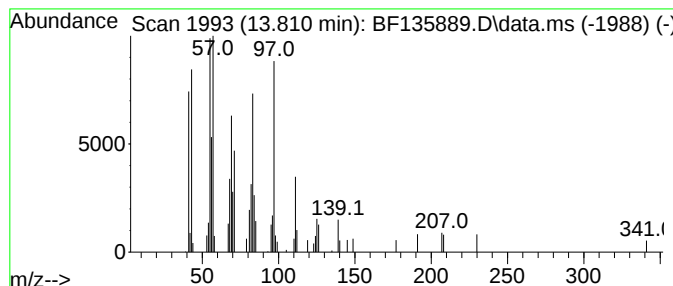
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Peak Number 4 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	5.62 ng	95424	Chrysene-d12	13.933

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Eicosene, (E)-	280	C20H40	074685-30-6	86
2		1-Docosene	308	C22H44	001599-67-3	86
3		10-Heneicosene (c,t)	294	C21H42	095008-11-0	86
4		1-Tricosanol	340	C23H48O	003133-01-5	86
5		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	83



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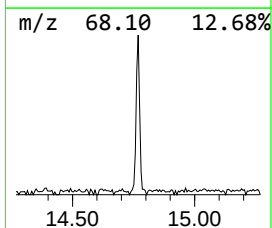
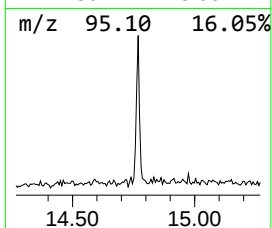
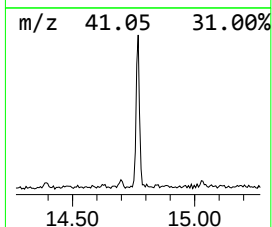
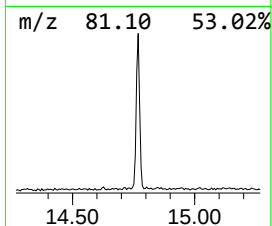
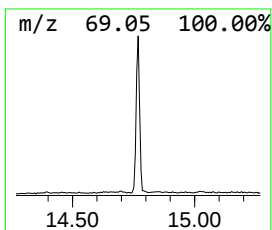
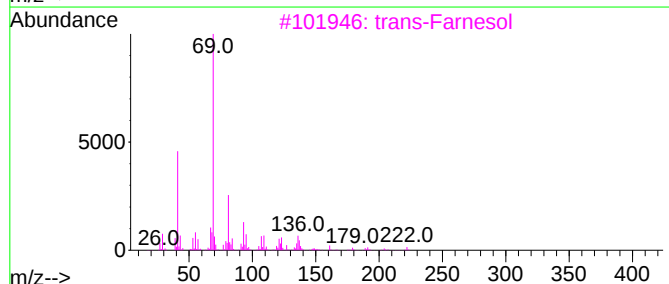
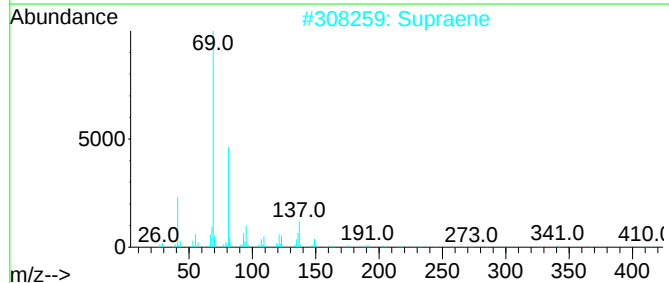
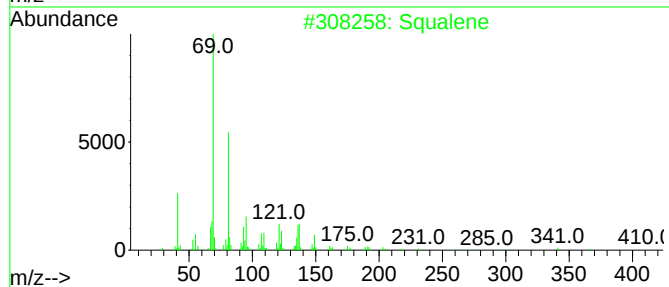
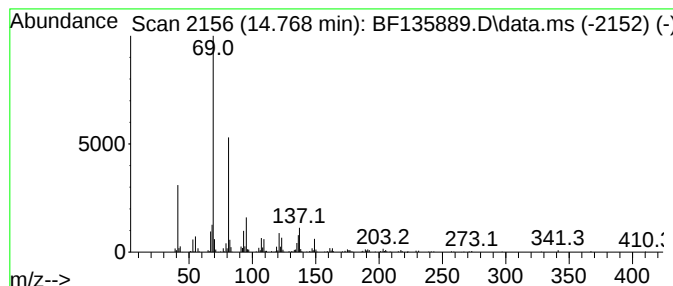
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Peak Number 5 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.769	17.94 ng	281936	Perylene-d12	15.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	95
2			Supraene	410	C30H50	007683-64-9	91
3			trans-Farnesol	222	C15H26O	000106-28-5	72
4			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52
5			4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.957	32.7	ng	622479	1	6.734	380468	20.0
n-Hexadecanoic ...	11.804	14.6	ng	359712	4	11.269	494280	20.0
Pentadecanoic acid	12.592	2.9	ng	70574	4	11.269	494280	20.0
5-Eicosene, (E)-	13.810	5.6	ng	95424	5	13.933	339452	20.0
Squalene	14.769	17.9	ng	281936	6	15.410	314260	20.0