

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112217\
 Data File : BF100871.D
 Acq On : 23 Nov 2017 13:19
 Operator : SJ/JU
 Sample : I6567-03
 Misc :
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 112017-TIDO-F-U-B

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:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.075	504	508	518	rBB	147181	155139	6.13%	1.119%
2	5.475	572	576	579	rBV	696344	617187	24.37%	4.452%
3	6.481	743	747	755	rBB	470954	433513	17.12%	3.127%
4	6.628	767	772	775	rBV	1290278	1145905	45.25%	8.266%
5	6.857	807	811	815	rBV	566293	443314	17.50%	3.198%
6	7.016	833	838	841	rBV	1920158	1684739	66.52%	12.153%
7	7.422	901	907	910	rBV	1214373	1380406	54.50%	9.958%
8	8.139	1024	1029	1032	rBV	712413	580741	22.93%	4.189%
9	9.216	1206	1212	1215	rBV	2656843	2532658	100.00%	18.270%
10	9.892	1321	1327	1331	rBV	665075	650468	25.68%	4.692%
11	10.563	1438	1441	1444	rVB	42014	28937	1.14%	0.209%
12	10.680	1457	1461	1465	rBV	920530	855499	33.78%	6.171%
13	11.380	1576	1580	1584	rBV	698629	567591	22.41%	4.094%
14	12.780	1814	1818	1821	rBV	54985	45332	1.79%	0.327%
15	12.968	1845	1850	1853	rBV	1948183	1810014	71.47%	13.057%
16	13.480	1934	1937	1941	rBV2	33254	30808	1.22%	0.222%
17	13.851	1997	2000	2004	rBV	46128	48730	1.92%	0.352%
18	14.021	2025	2029	2032	rBV	412175	382495	15.10%	2.759%
19	15.492	2273	2279	2285	rBV	342950	436017	17.22%	3.145%
20	16.439	2435	2440	2447	rVB3	19264	33181	1.31%	0.239%

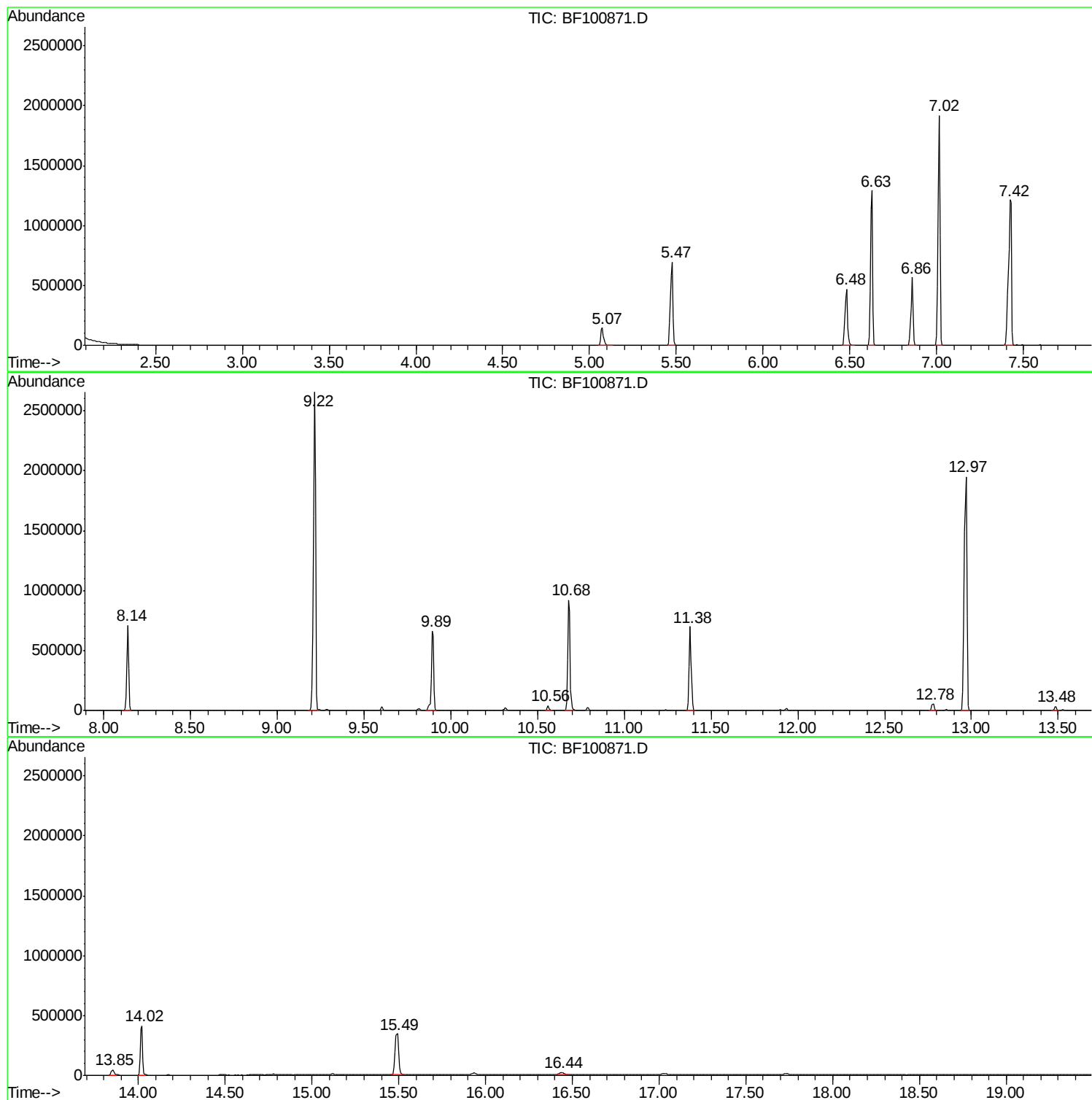
Sum of corrected areas: 13862674

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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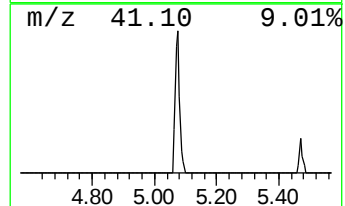
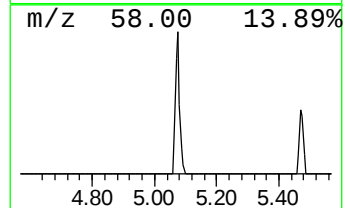
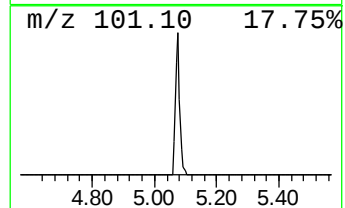
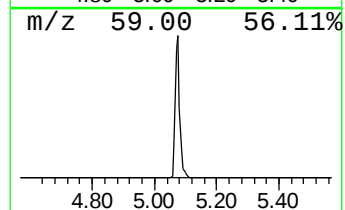
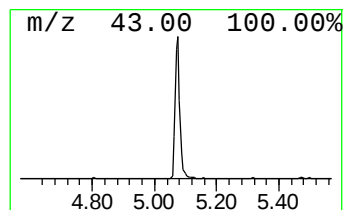
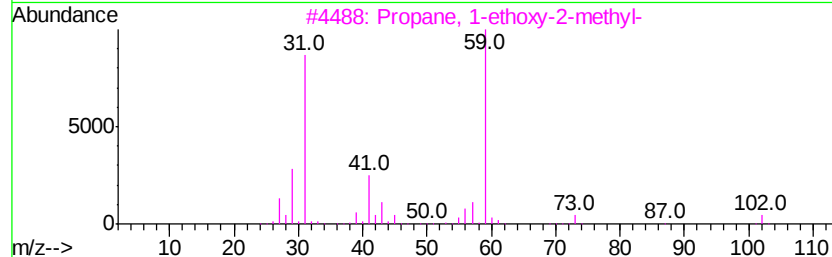
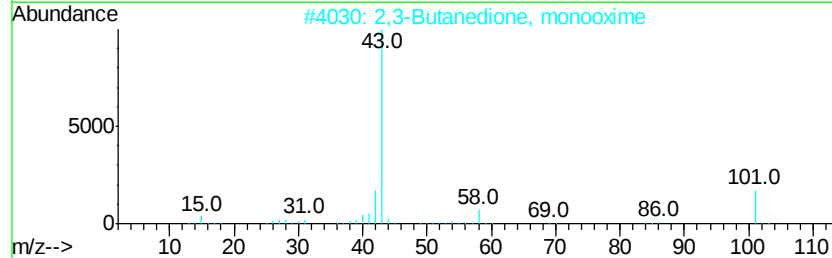
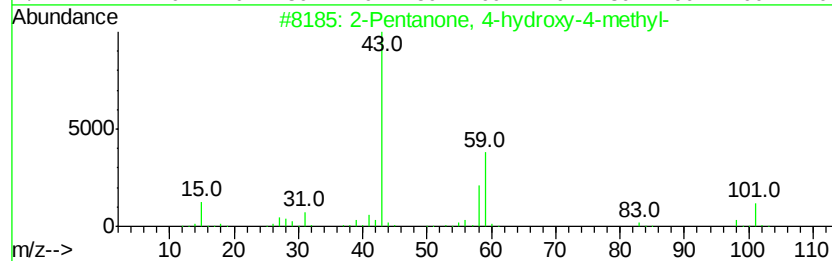
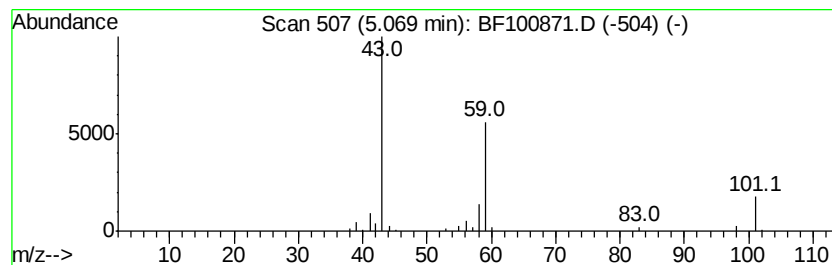
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	7.00 ng	155139	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9
5			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9



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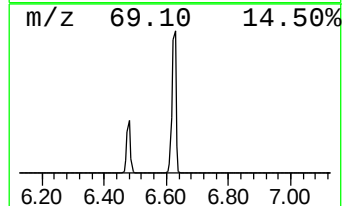
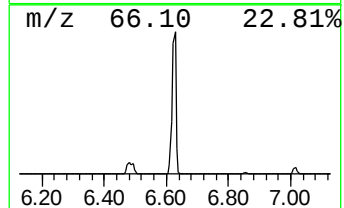
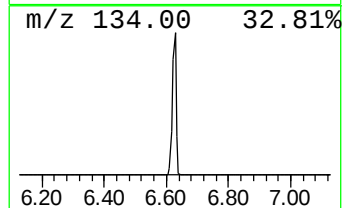
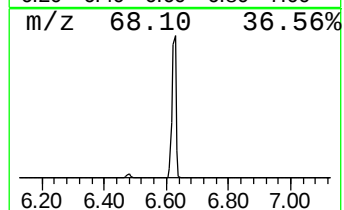
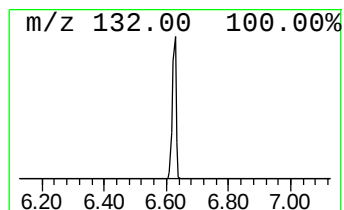
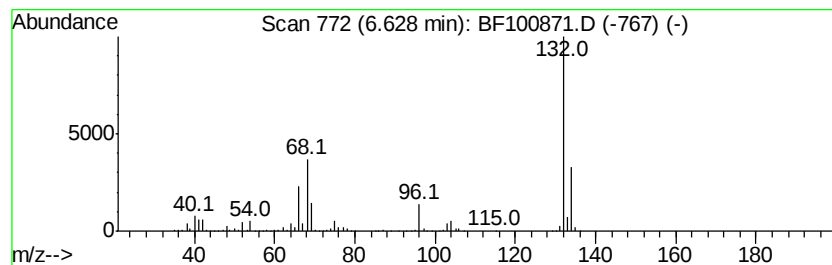
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TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	51.70 ng	1145910	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	12
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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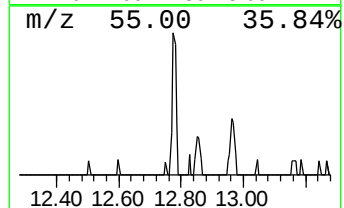
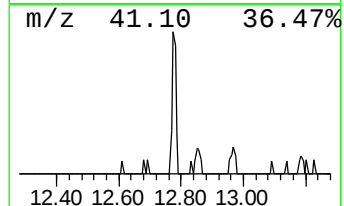
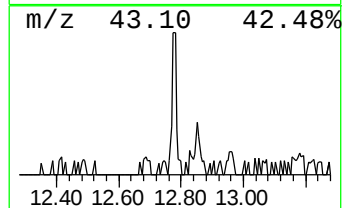
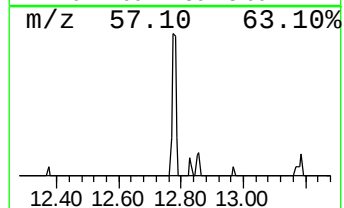
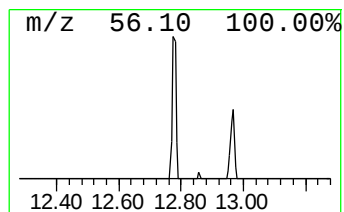
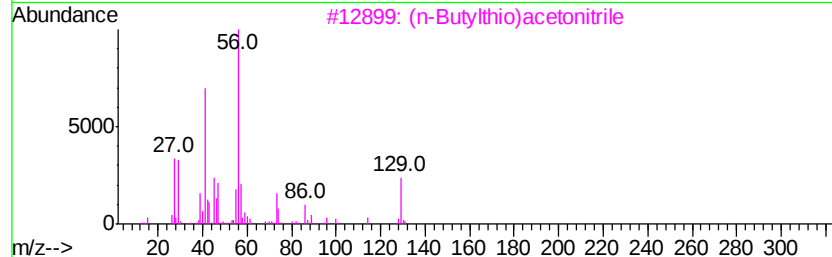
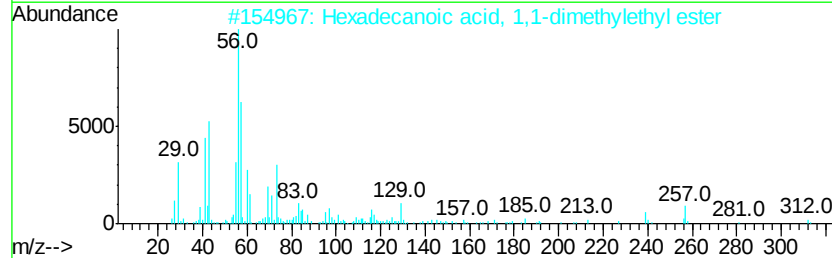
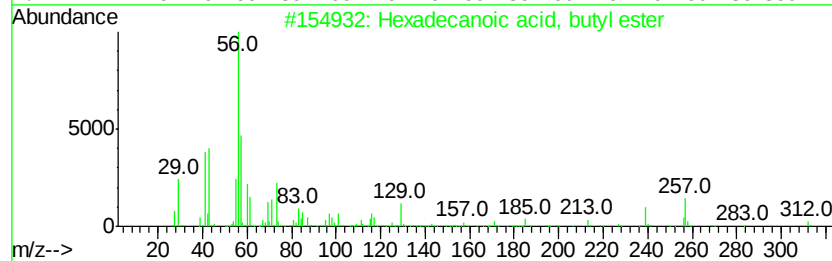
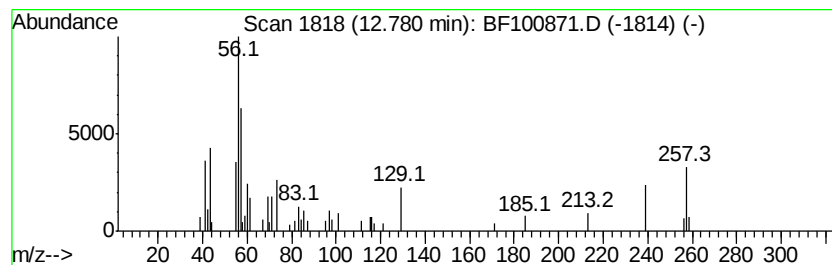
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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	2.37 ng	45332	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	74
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	58
3		(n-Butylthio)acetonitrile	129	C6H11NS	071037-08-6	46
4		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	38
5		Nipecotic acid	129	C6H11NO2	000498-95-3	38



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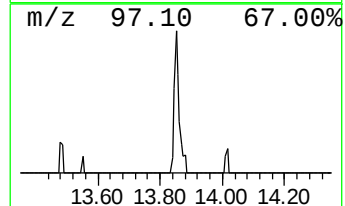
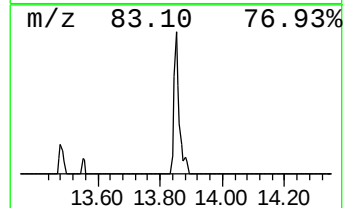
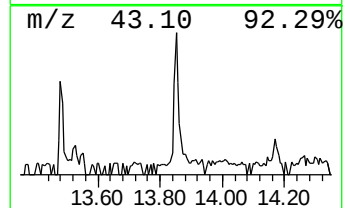
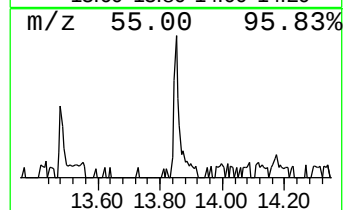
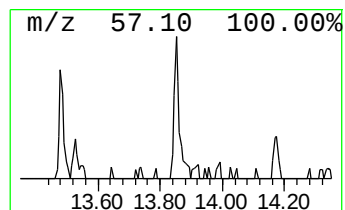
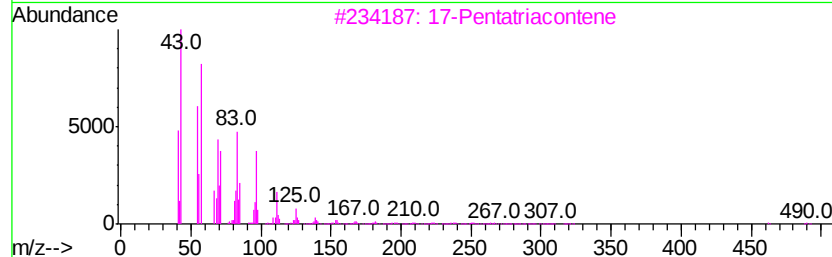
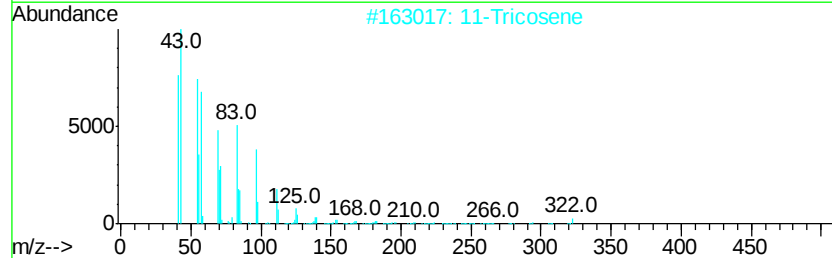
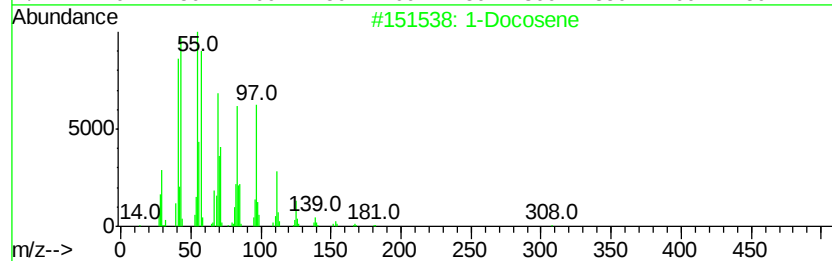
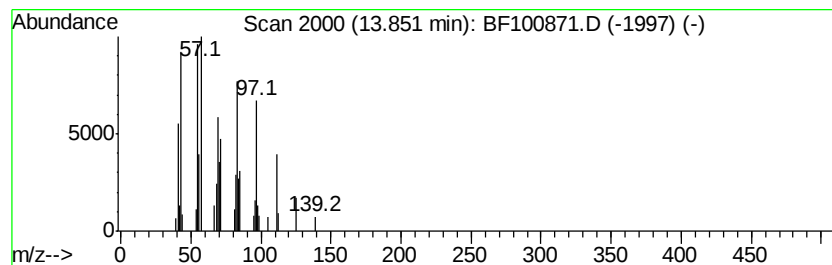
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Peak Number 5 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	2.55 ng	48730	Chrysene-d12	14.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene		308	C22H44	001599-67-3	86
2	11-Tricosene		322	C23H46	052078-56-5	86
3	17-Pentatriacontene		491	C35H70	006971-40-0	86
4	Carbonic acid, isobutyl octadecyl...		370	C23H46O3	1000314-61-5	80
5	5-Eicosene, (E)-		280	C20H40	074685-30-6	74



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.07	7.0	ng	155139	1	6.86	443314	20.0
unknown6.63	6.63	51.7	ng	1145910	1	6.86	443314	20.0
Hexadecanoic acid...	12.78	2.4	ng	45332	5	14.02	382495	20.0
1-Docosene	13.85	2.5	ng	48730	5	14.02	382495	20.0