

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110323\
 Data File : BF136129.D
 Acq On : 03 Nov 2023 17:39
 Operator : CG\JU
 Sample : 05141-05
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PE-5

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-BF103023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136129.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.051	498	504	513	rVB	59680	75021	2.81%	0.425%
2	5.451	566	572	575	rBV	2275377	2183326	81.73%	12.373%
3	6.451	736	742	745	rBV	2113896	2165119	81.05%	12.270%
4	6.816	801	804	808	rBV	756943	640337	23.97%	3.629%
5	7.381	895	900	903	rBV	1749455	1436986	53.79%	8.144%
6	8.098	1018	1022	1025	rBV	1112299	831135	31.11%	4.710%
7	9.180	1202	1206	1209	rBV	3347514	2671232	100.00%	15.138%
8	9.857	1317	1321	1324	rBV	1205372	907349	33.97%	5.142%
9	10.645	1451	1455	1459	rBV	1729554	1537954	57.57%	8.716%
10	11.345	1571	1574	1577	rBV	896182	825569	30.91%	4.679%
11	11.369	1577	1578	1582	rVB	72901	50032	1.87%	0.284%
12	11.886	1662	1666	1670	rBV2	139567	128854	4.82%	0.730%
13	12.563	1778	1781	1785	rBV	90676	82625	3.09%	0.468%
14	12.680	1796	1801	1806	rBV	30119	40597	1.52%	0.230%
15	12.792	1813	1820	1824	rBV	71269	81289	3.04%	0.461%
16	12.951	1842	1847	1850	rBV	2613726	2252801	84.34%	12.767%
17	13.880	2000	2005	2018	rBV8	33881	115045	4.31%	0.652%
18	14.004	2021	2026	2029	rBV	766792	706596	26.45%	4.004%
19	15.051	2200	2204	2208	rBV2	39330	63870	2.39%	0.362%
20	15.421	2263	2267	2273	rVB	30575	38198	1.43%	0.216%
21	15.492	2273	2279	2287	rBV	651819	811523	30.38%	4.599%

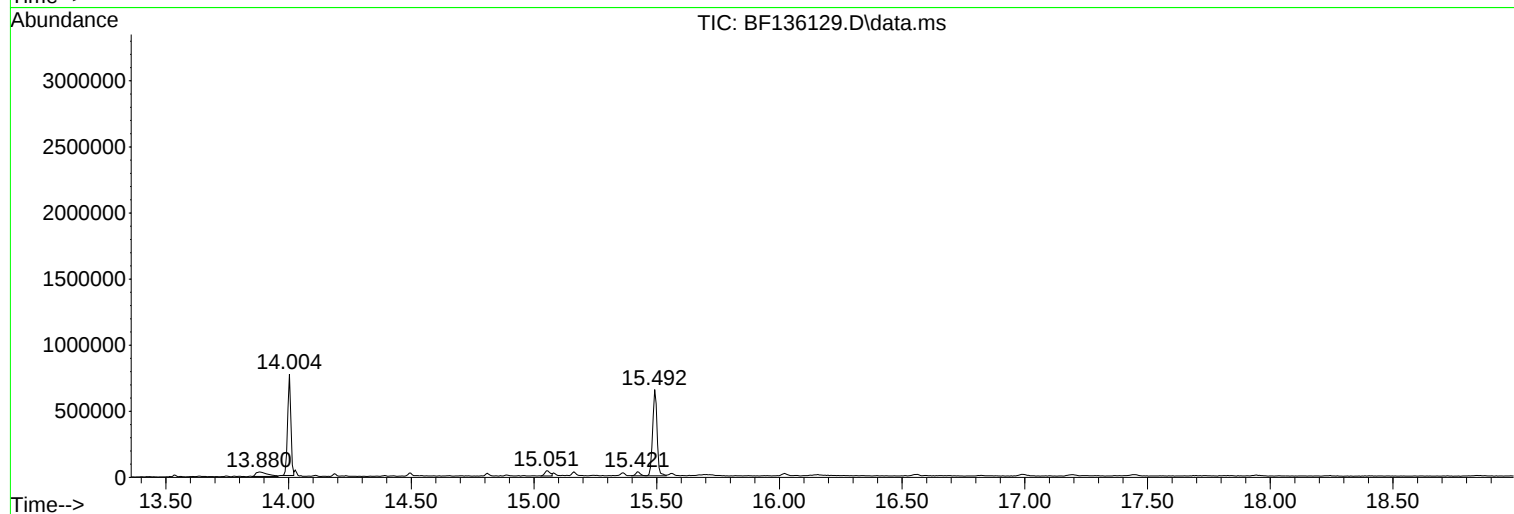
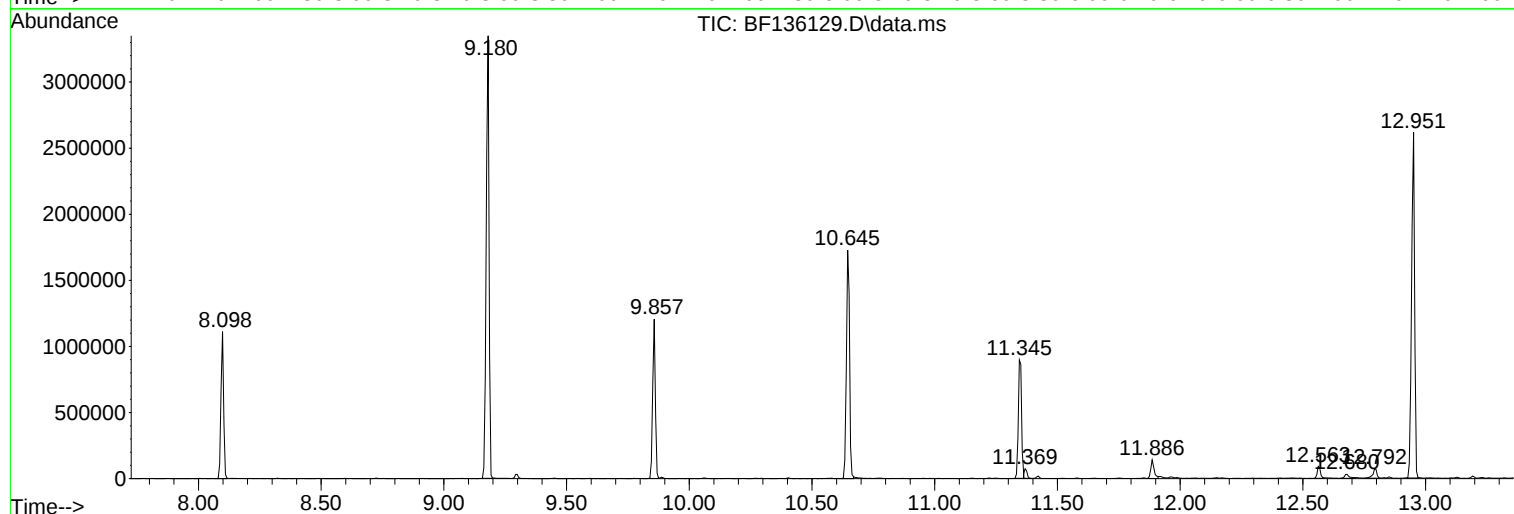
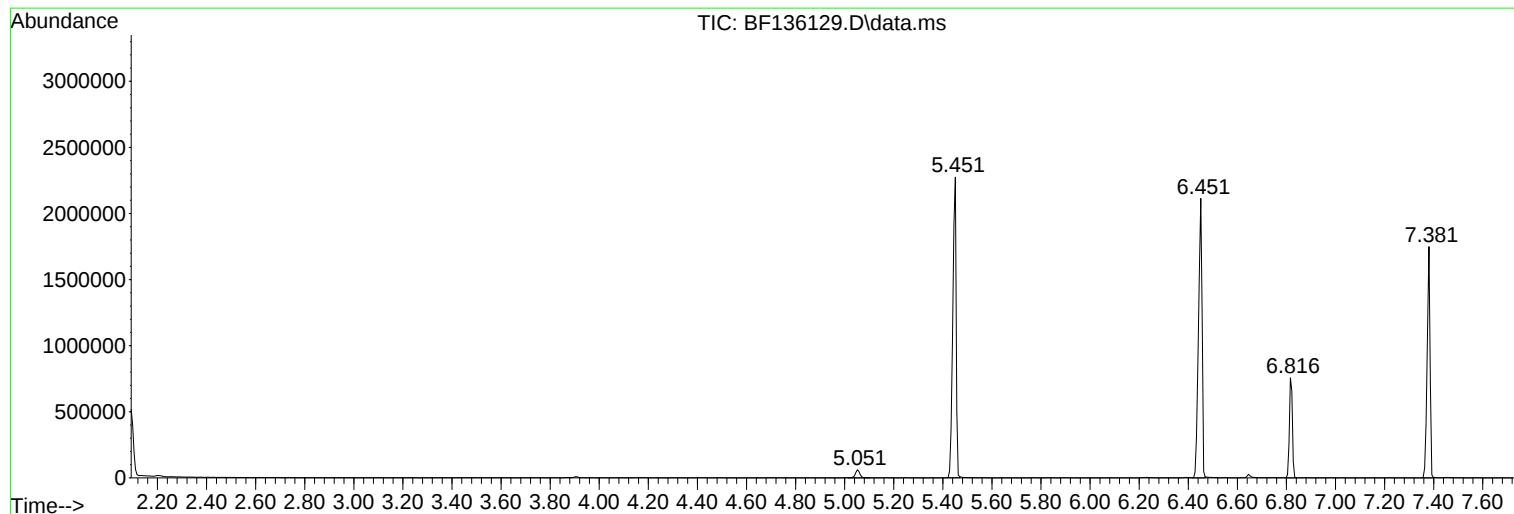
Sum of corrected areas: 17645458

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.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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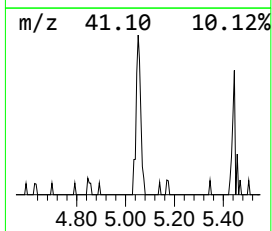
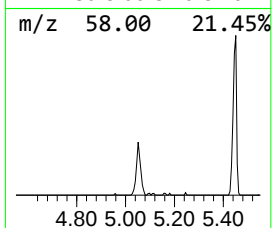
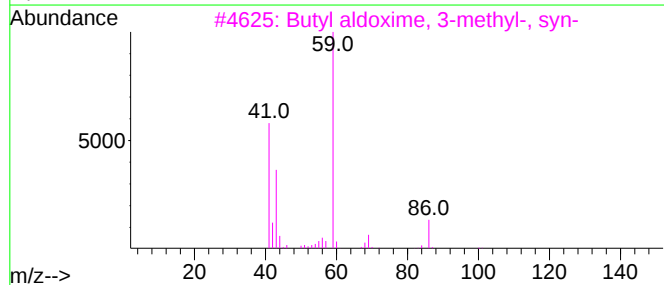
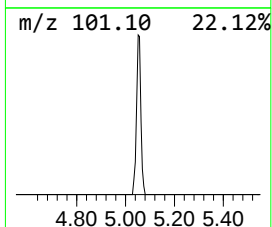
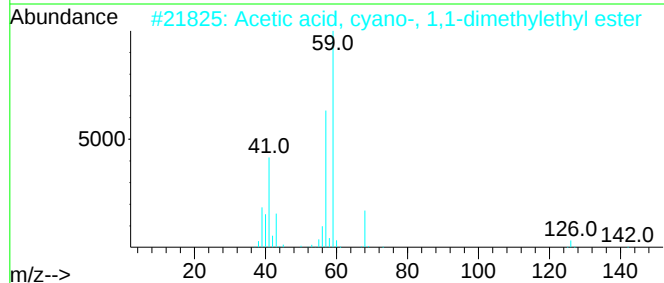
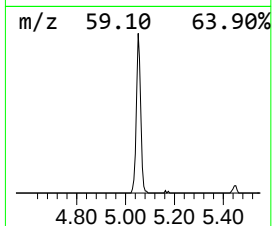
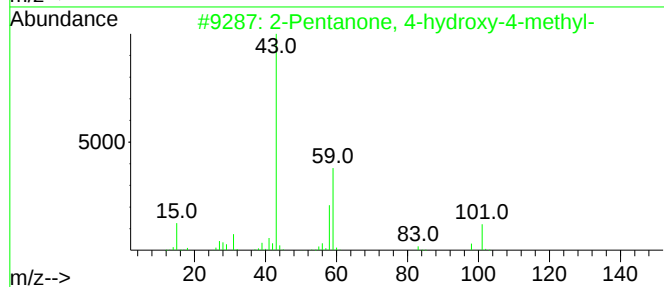
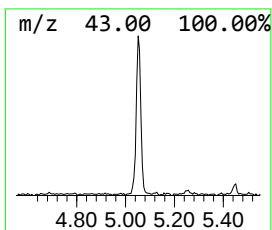
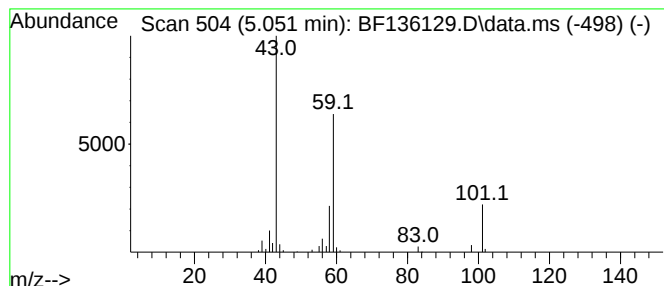
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.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.
5.051	2.34 ng	75021	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	16		
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	16		
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	12		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		



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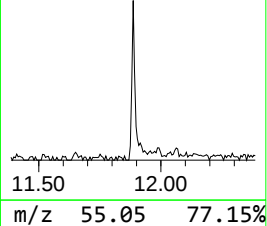
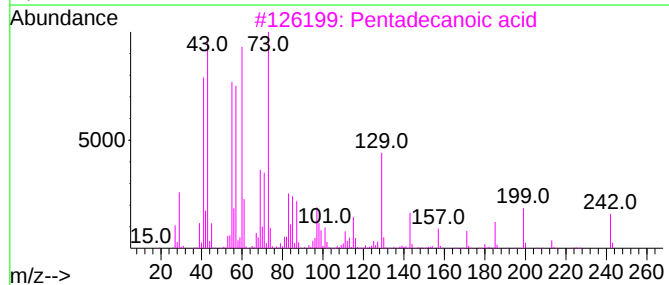
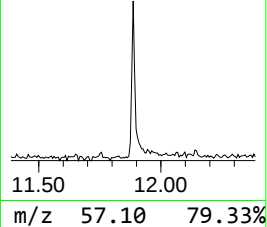
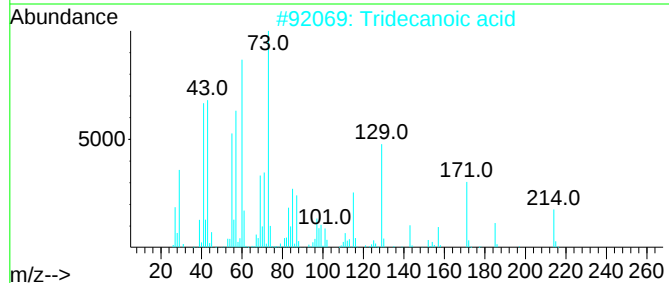
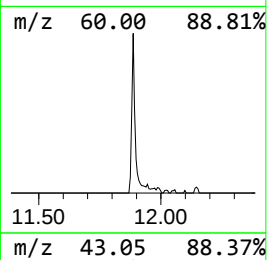
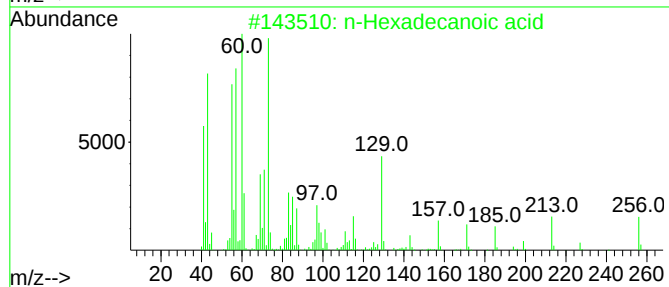
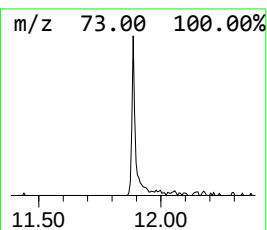
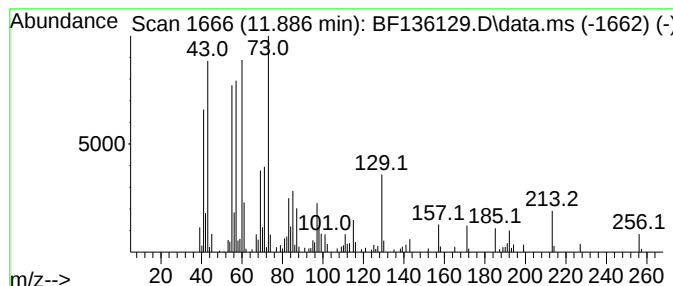
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	3.12 ng	128854	Phenanthrene-d10	11.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	92
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60



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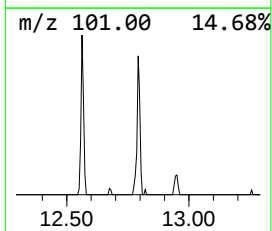
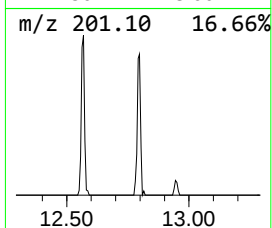
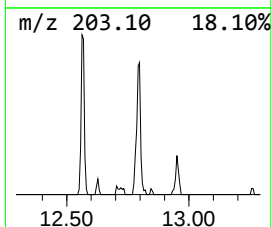
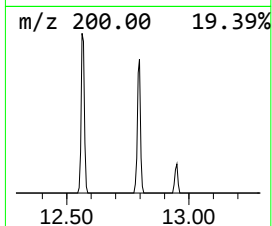
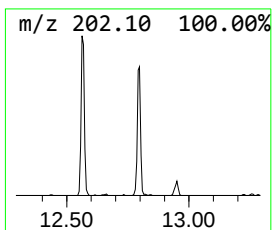
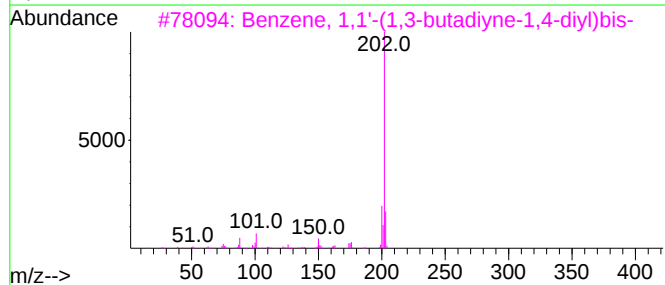
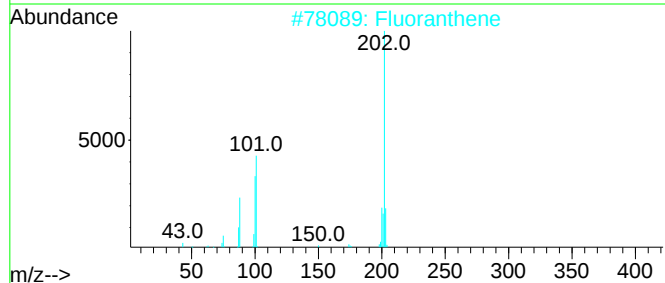
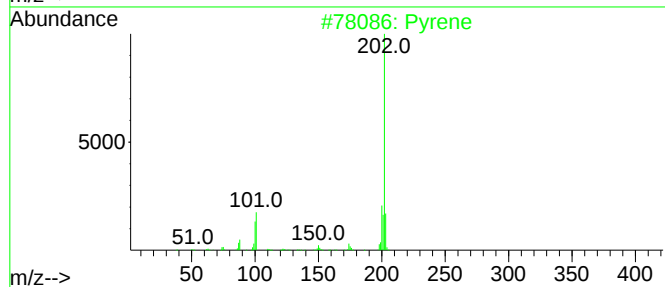
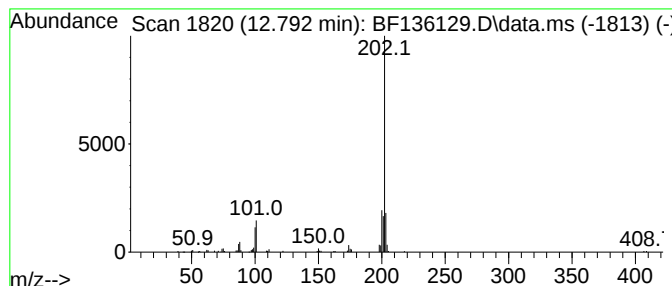
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Peak Number 3 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.792	2.30 ng	81289	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene	202	C16H10	000129-00-0	94
2			Fluoranthene	202	C16H10	000206-44-0	93
3			Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	64
4			Anthracene, 9-(2-nitroethenyl)-	249	C16H11NO2	058349-77-2	39
5			4-Methoxy-naphthalene-1-carboxyl...	202	C12H10O3	1000317-85-4	38



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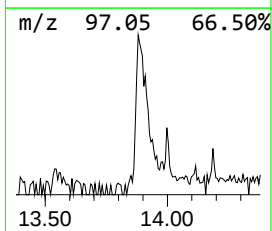
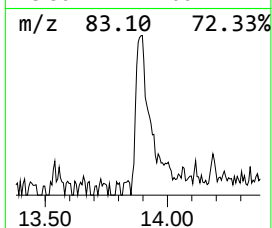
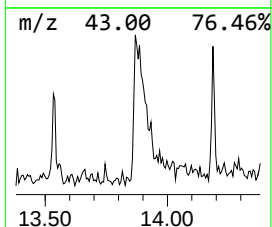
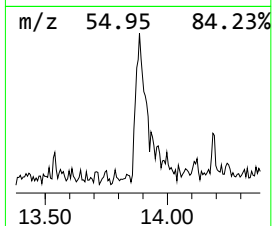
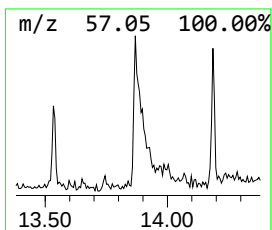
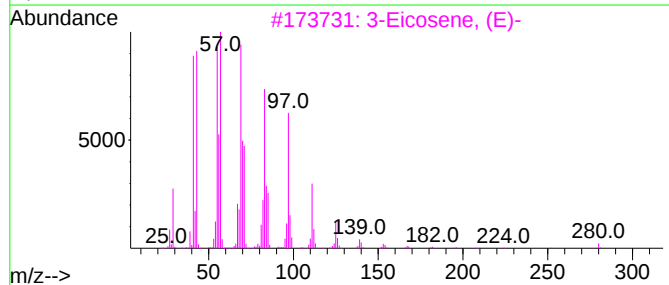
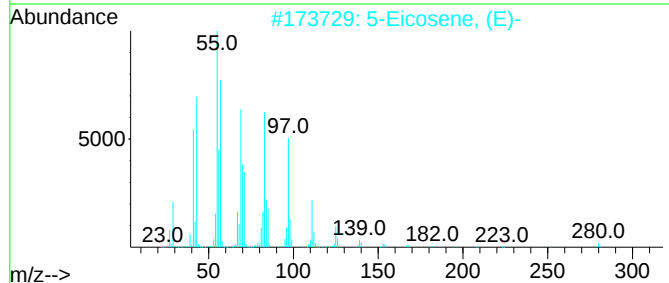
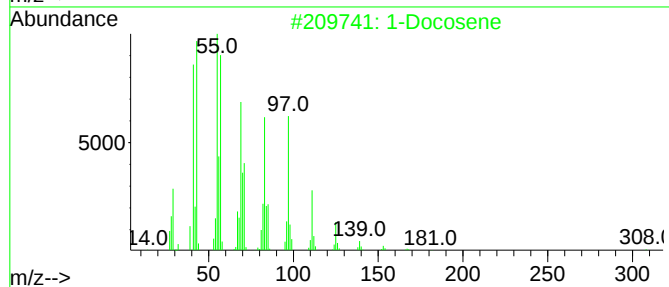
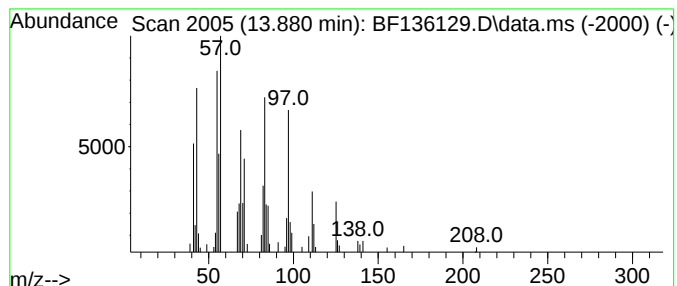
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Peak Number 4 1-Docosene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	3.26 ng	115045	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	91
2	5-Eicosene, (E)-			280	C20H40	074685-30-6	90
3	3-Eicosene, (E)-			280	C20H40	074685-33-9	90
4	11-Tricosene			322	C23H46	052078-56-5	86
5	Octadecyl trifluoroacetate			366	C20H37F3O2	079392-43-1	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.051	2.3	ng	75021	1	6.816	640337	20.0
n-Hexadecanoic ...	11.886	3.1	ng	128854	4	11.351	825569	20.0
Benzene, 1,1'-(...	12.792	2.3	ng	81289	5	14.004	706596	20.0
1-Docosene	13.880	3.3	ng	115045	5	14.004	706596	20.0