

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
 Data File : BF096548.D
 Acq On : 6 Jul 2017 22:05
 Operator : SJ/MA
 Sample : I3972-06
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B5-14-14.5

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:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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	4.910	475	480	490	rVB	277249	399928	15.27%	1.880%
2	5.334	547	552	555	rBV	2566411	2579471	98.47%	12.125%
3	6.357	720	726	739	rVB	2309404	2619510	100.00%	12.313%
4	6.486	743	748	751	rBV	2590630	2494172	95.22%	11.724%
5	6.710	783	786	790	rBV	702041	626948	23.93%	2.947%
6	6.869	809	813	817	rBV	2023327	1923480	73.43%	9.041%
7	7.275	876	882	885	rBV	1690841	1532029	58.49%	7.201%
8	7.992	1000	1004	1008	rBV	904494	797489	30.44%	3.749%
9	9.075	1183	1188	1191	rBV	2724715	2414118	92.16%	11.348%
10	9.463	1251	1254	1258	rBV	246922	204653	7.81%	0.962%
11	9.745	1298	1302	1306	rBV	768658	723350	27.61%	3.400%
12	10.192	1375	1378	1381	rVB	45547	37021	1.41%	0.174%
13	10.533	1432	1436	1445	rVB	1169191	1069483	40.83%	5.027%
14	10.663	1456	1458	1465	rBV	48323	55665	2.13%	0.262%
15	11.227	1550	1554	1558	rBV	679313	552824	21.10%	2.599%
16	11.468	1591	1595	1600	rVB	32043	33308	1.27%	0.157%
17	12.286	1730	1734	1740	rBV	133759	132987	5.08%	0.625%
18	12.815	1820	1824	1827	rBV	1780753	1650922	63.02%	7.760%
19	13.033	1857	1861	1864	rBV	34605	36494	1.39%	0.172%
20	13.268	1898	1901	1906	rBV	46075	41506	1.58%	0.195%
21	13.721	1972	1978	1986	rBV	127181	163505	6.24%	0.769%
22	13.862	1998	2002	2005	rBV	686980	640801	24.46%	3.012%
23	14.715	2144	2147	2152	rVB	51695	49214	1.88%	0.231%
24	15.274	2237	2242	2246	rBV	413479	495431	18.91%	2.329%

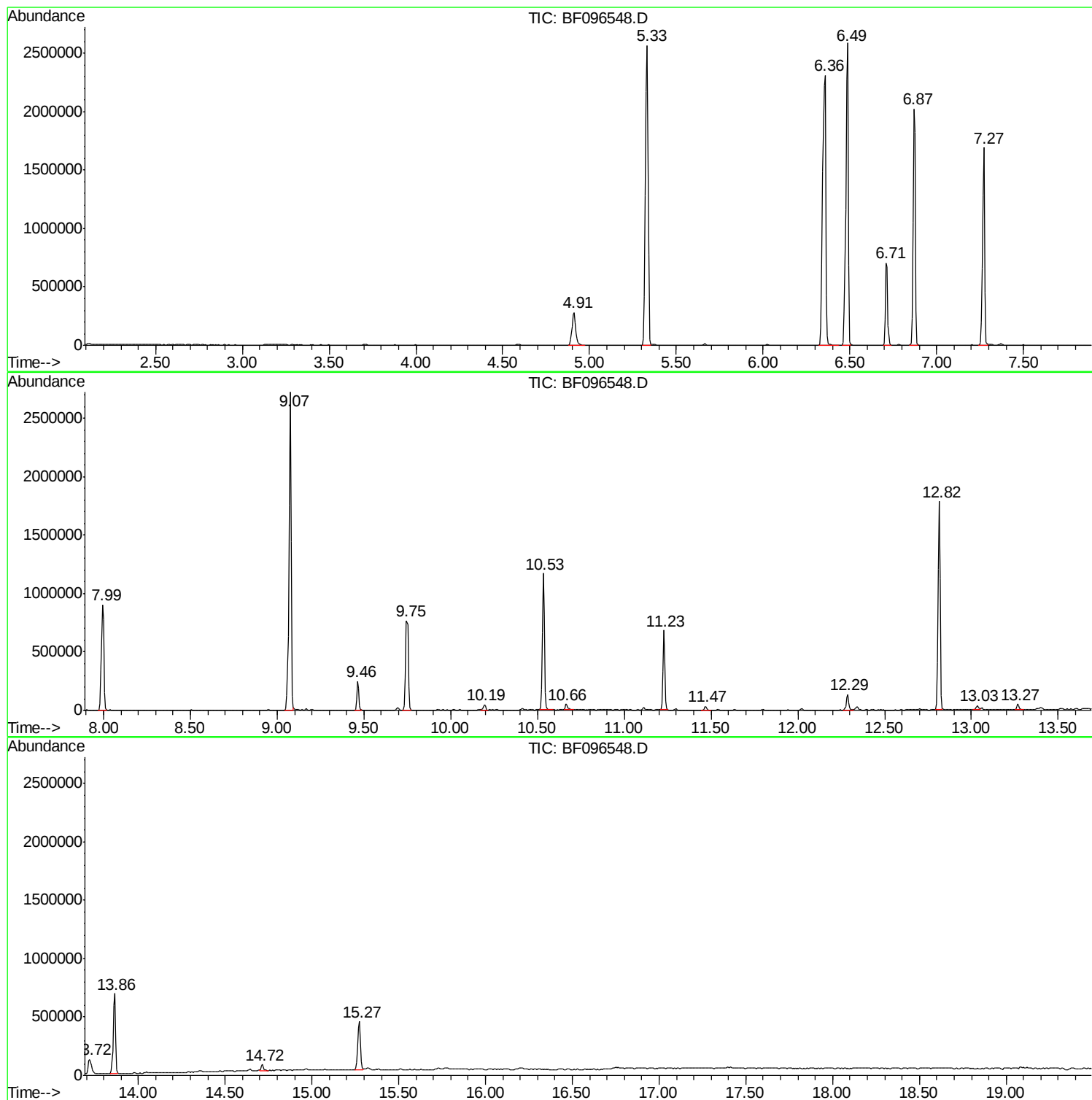
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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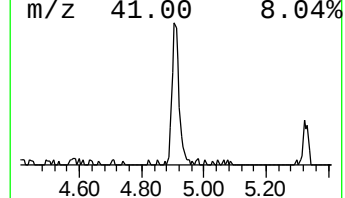
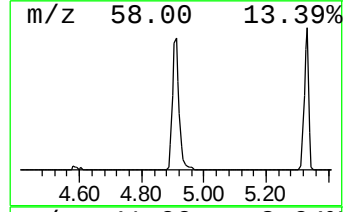
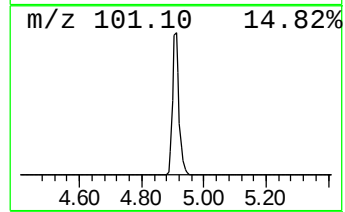
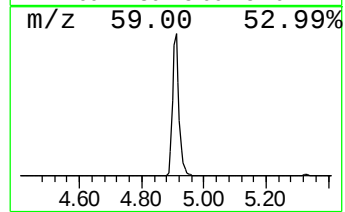
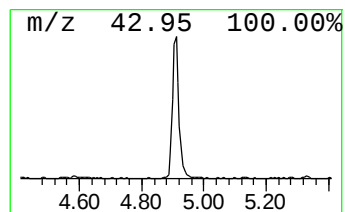
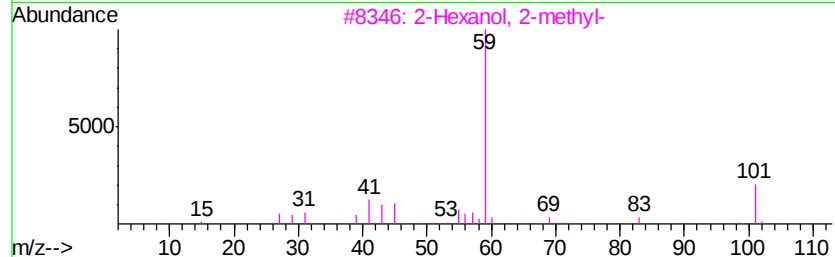
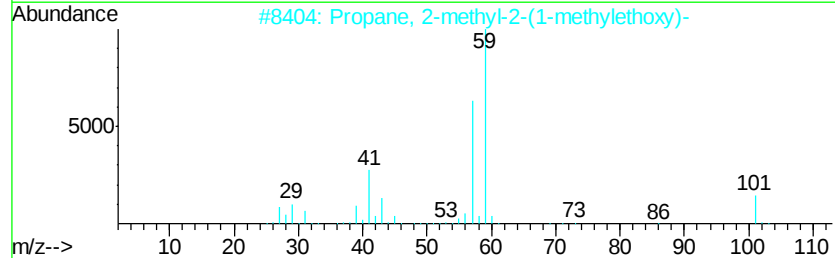
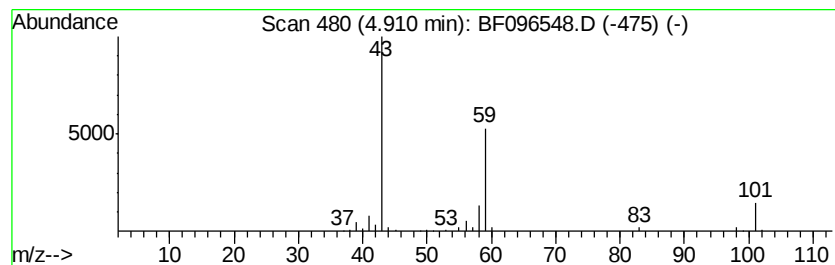
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	12.76 ng	399928	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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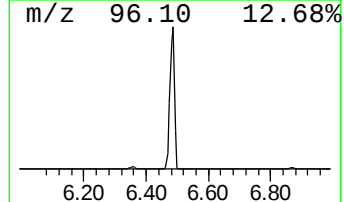
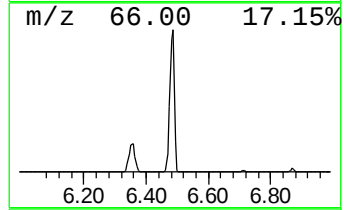
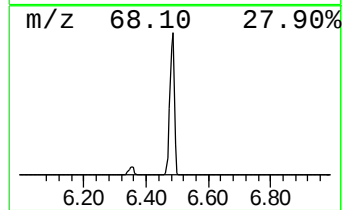
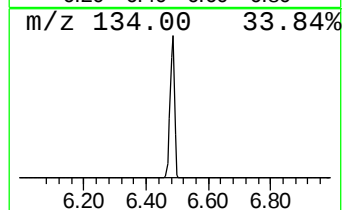
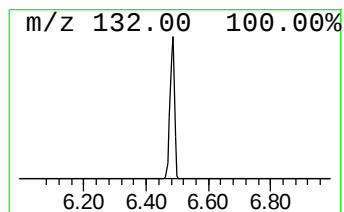
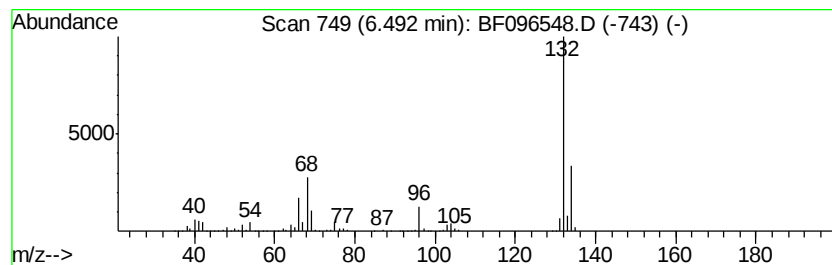
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	79.57 ng	2494170	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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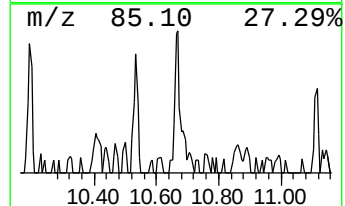
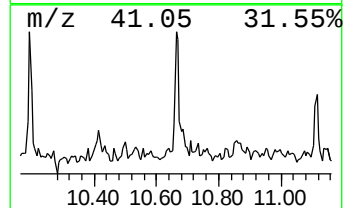
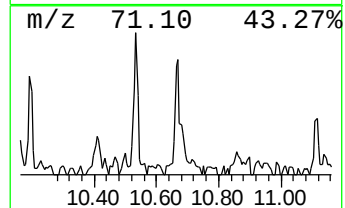
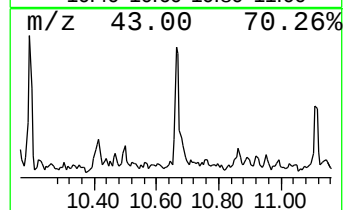
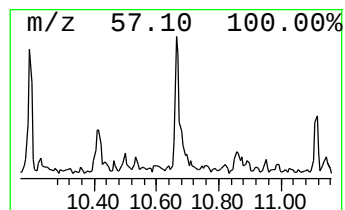
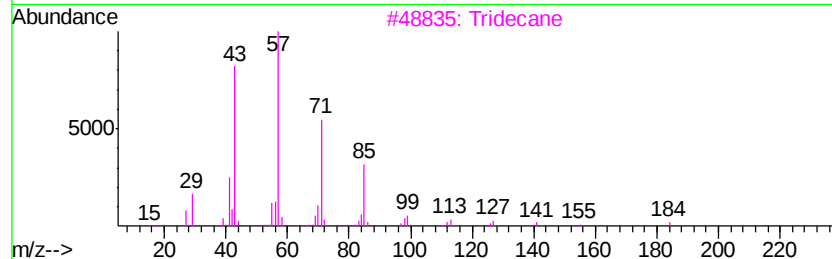
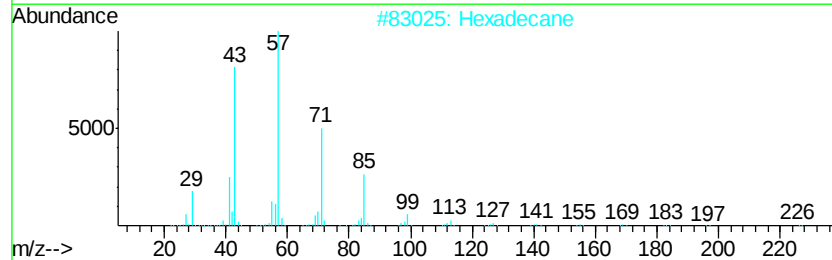
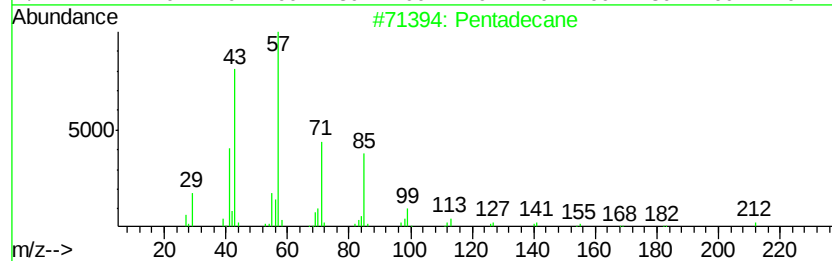
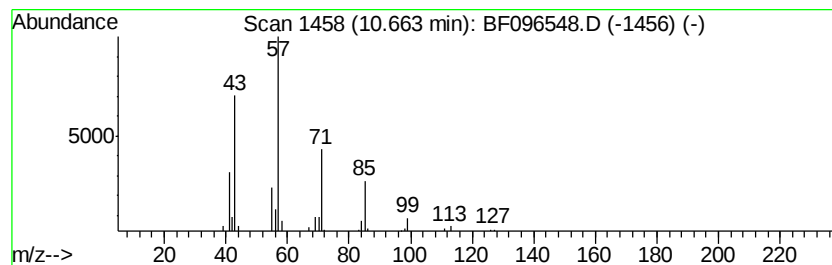
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Peak Number 4 Pentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	2.01 ng	55665	Phenanthrene-d10	11.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane		212	C15H32	000629-62-9	86
2	Hexadecane		226	C16H34	000544-76-3	86
3	Tridecane		184	C13H28	000629-50-5	86
4	Tetradecane		198	C14H30	000629-59-4	78
5	Nonadecane		268	C19H40	000629-92-5	64



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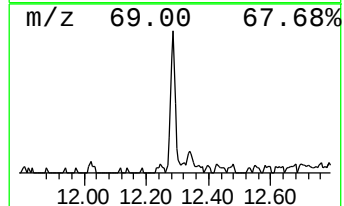
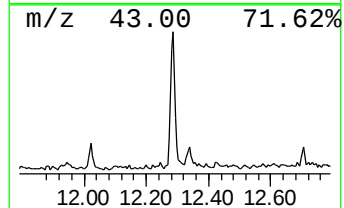
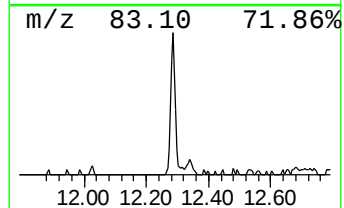
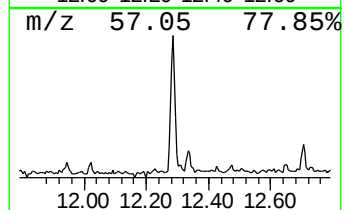
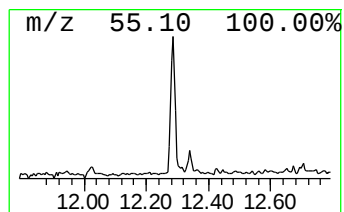
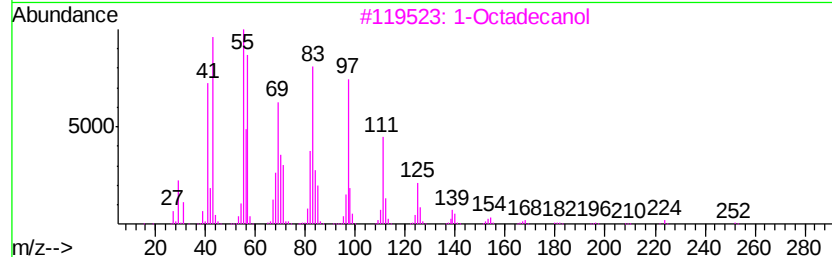
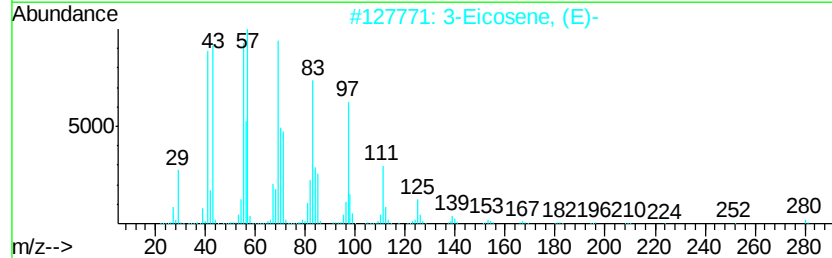
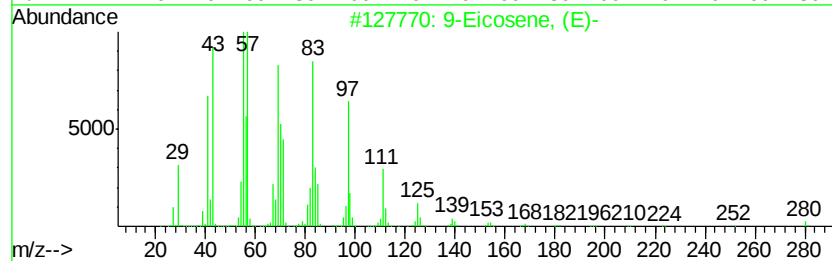
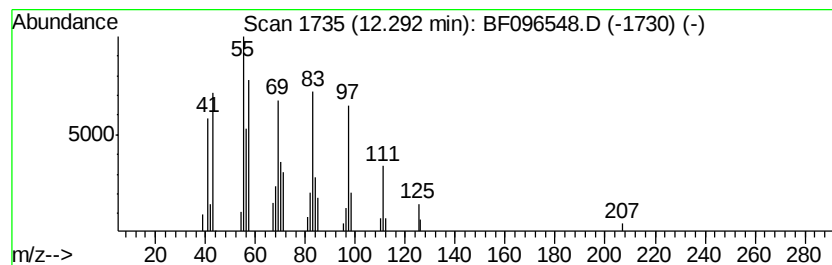
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Peak Number 5 9-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	4.81 ng	132987	Phenanthrene-d10	11.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Eicosene, (E)-	280	C20H40	074685-29-3	91
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3		1-Octadecanol	270	C18H38O	000112-92-5	91
4		1-Nonadecene	266	C19H38	018435-45-5	91
5		5-Eicosene, (E)-	280	C20H40	074685-30-6	90



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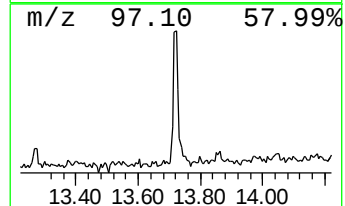
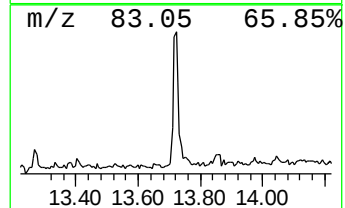
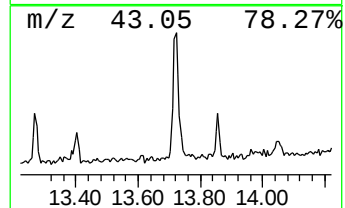
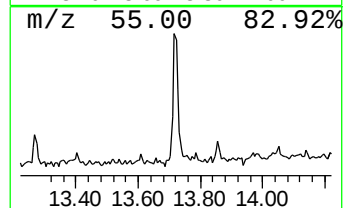
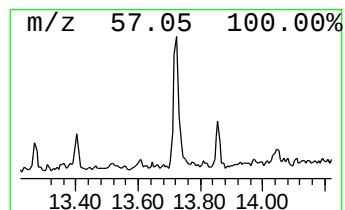
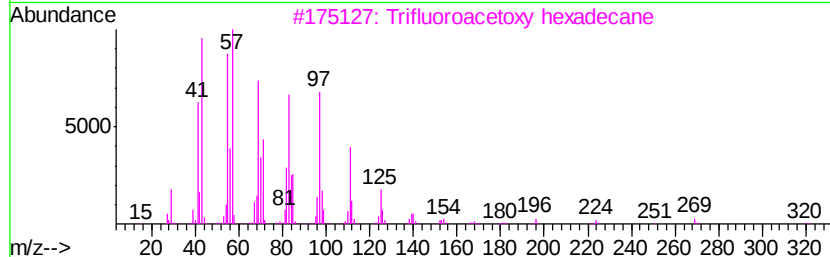
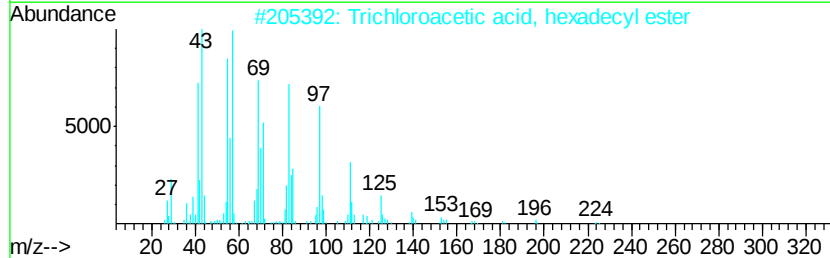
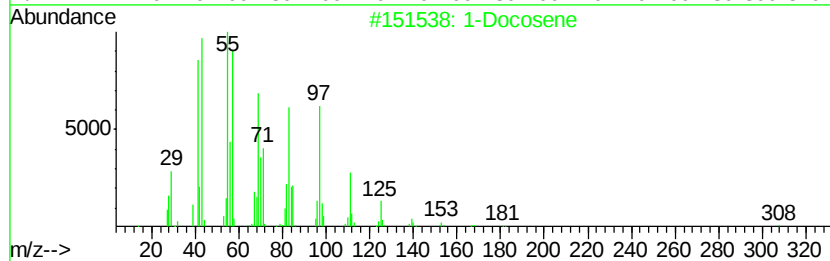
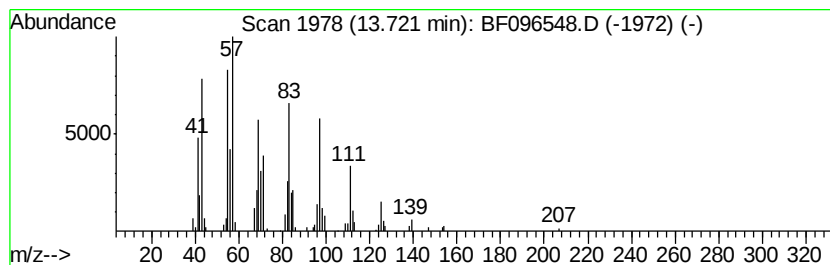
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Peak Number 6 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	5.10 ng	163505	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	95
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5		Octacosanol	410	C28H58O	000557-61-9	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.91	12.8	ng	399928	1	6.72	626948	20.0
unknown6.49	6.49	79.6	ng	2494170	1	6.72	626948	20.0
Pentadecane	10.66	2.0	ng	55665	4	11.23	552824	20.0
9-Eicosene, (E)-	12.29	4.8	ng	132987	4	11.23	552824	20.0
1-Docosene	13.72	5.1	ng	163505	5	13.86	640801	20.0