

Data Path : Z:\HPCHEM1\BNA_F\Data\BF071217\
 Data File : BF096695.D
 Acq On : 12 Jul 2017 16:51
 Operator : SJ/JU
 Sample : I4126-03
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PP-WW-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:\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	4.851	466	470	484	rVB	307740	442938	17.08%	2.053%
2	5.281	538	543	546	rBV	2458016	2441198	94.16%	11.313%
3	6.310	713	718	721	rBV	2425406	2592656	100.00%	12.015%
4	6.440	735	740	743	rBV	2588470	2509432	96.79%	11.629%
5	6.663	775	778	782	rBV	814414	751231	28.98%	3.481%
6	6.822	801	805	809	rBV	1920321	1854119	71.51%	8.592%
7	7.228	869	874	877	rBV	1600091	1584679	61.12%	7.344%
8	7.945	992	996	1000	rBV	993109	959868	37.02%	4.448%
9	9.028	1175	1180	1183	rBV	2808759	2577473	99.41%	11.945%
10	9.416	1243	1246	1250	rBV	211185	180938	6.98%	0.839%
11	9.698	1289	1294	1298	rBV2	1110718	925372	35.69%	4.288%
12	10.145	1367	1370	1373	rVB	51064	40377	1.56%	0.187%
13	10.486	1423	1428	1431	rBV	1307460	1218950	47.02%	5.649%
14	10.616	1447	1450	1458	rBV	59688	66294	2.56%	0.307%
15	11.175	1541	1545	1549	rVB	863242	746473	28.79%	3.459%
16	12.763	1810	1815	1818	rBV	1560855	1412079	54.46%	6.544%
17	13.669	1962	1969	1974	rBV2	151639	181753	7.01%	0.842%
18	13.804	1988	1992	1996	rBV	626488	565683	21.82%	2.622%
19	15.198	2224	2229	2234	rBV	423748	498600	19.23%	2.311%
20	15.686	2310	2312	2318	rVB7	20510	28335	1.09%	0.131%

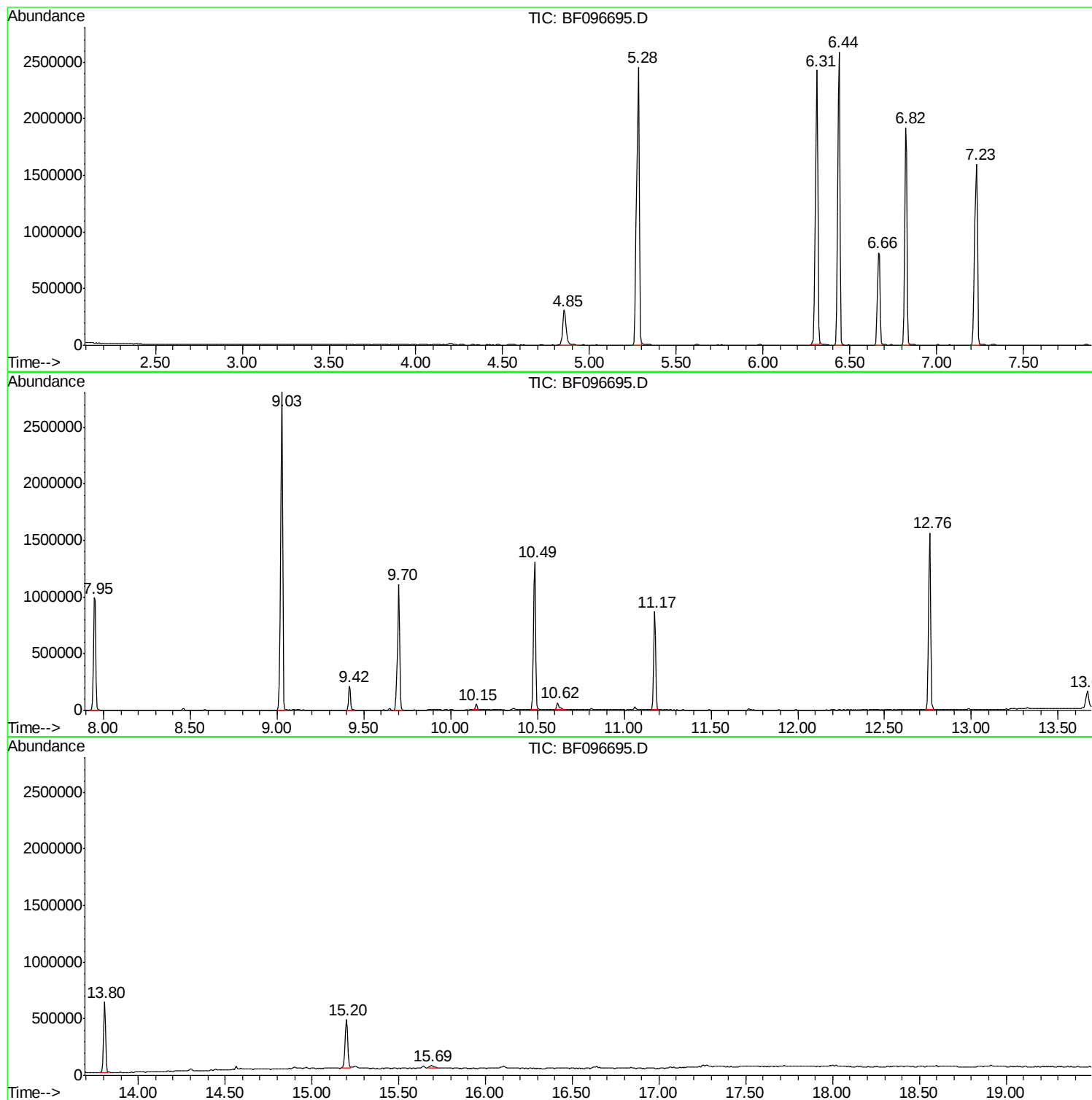
Sum of corrected areas: 21578448

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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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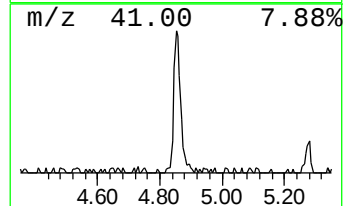
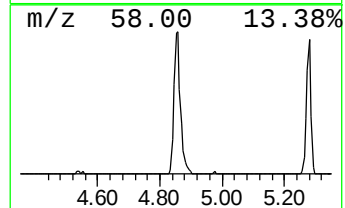
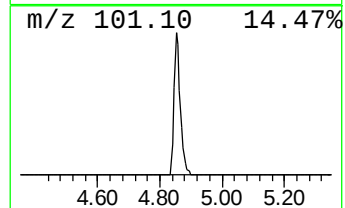
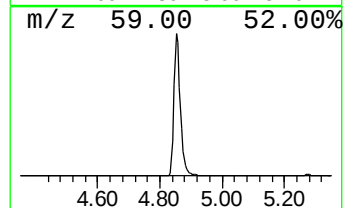
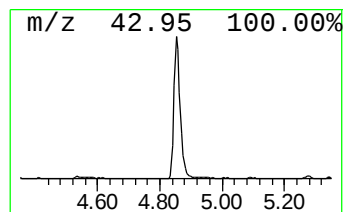
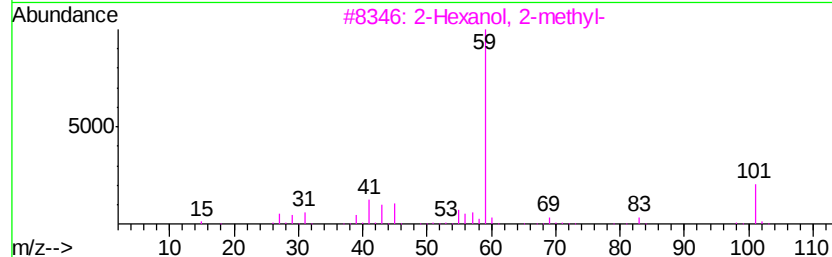
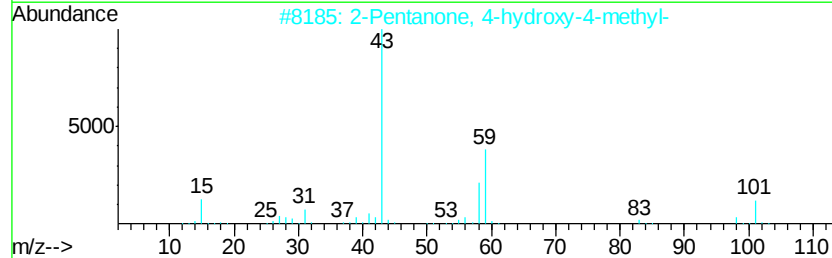
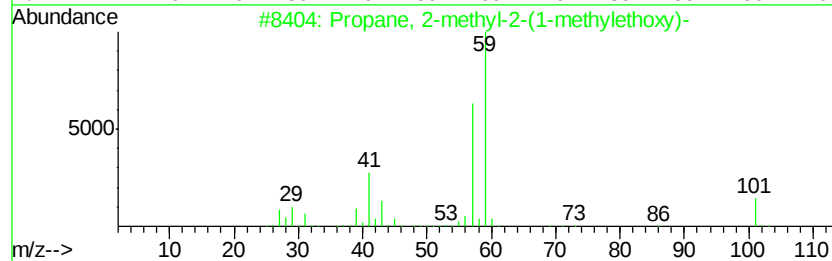
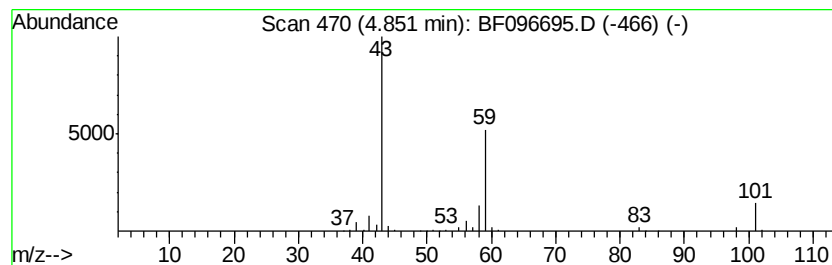
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown4.85 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	11.79 ng	442938	1,4-Dichlorobenzene-d4	6.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		3-Hexanol	102	C6H14O	000623-37-0	33
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28



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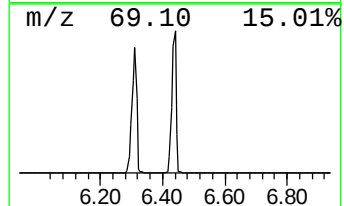
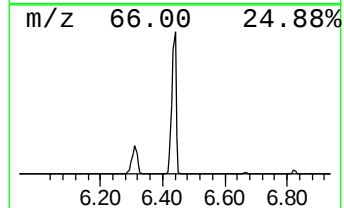
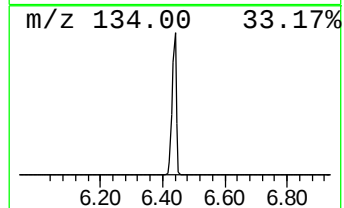
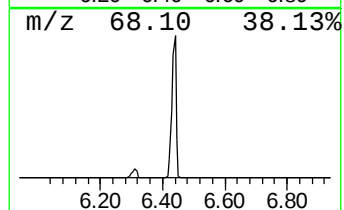
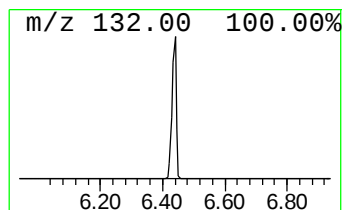
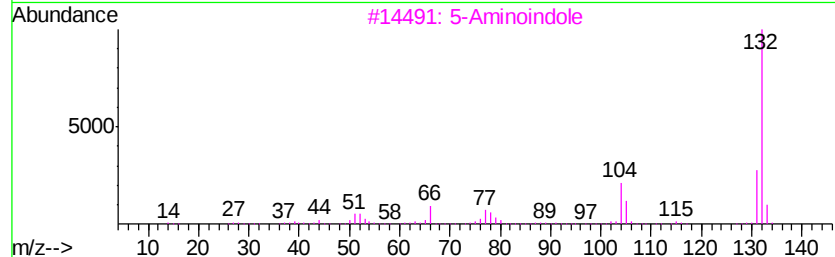
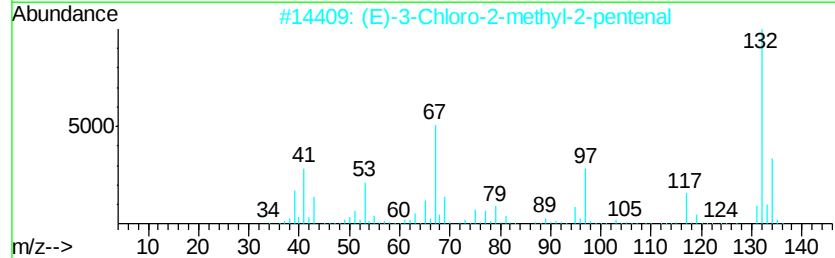
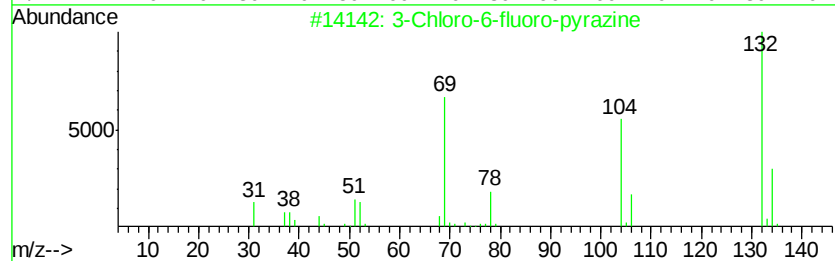
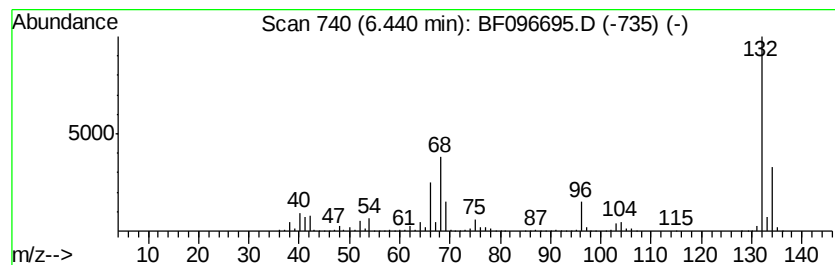
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Peak Number 2 unknown6.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	66.81 ng	2509430	1,4-Dichlorobenzene-d4	6.67

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		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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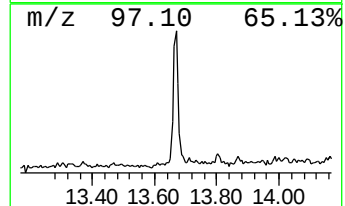
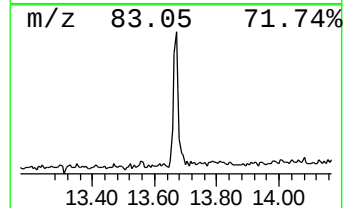
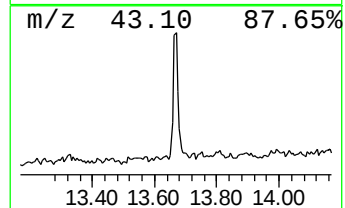
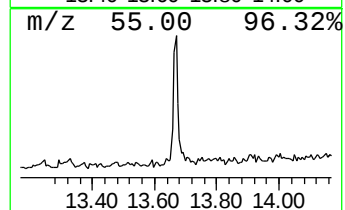
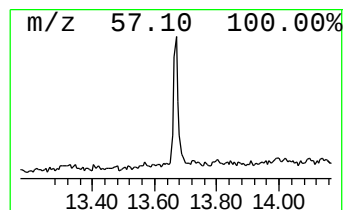
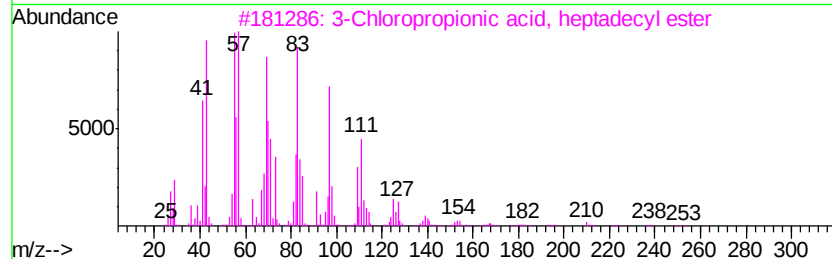
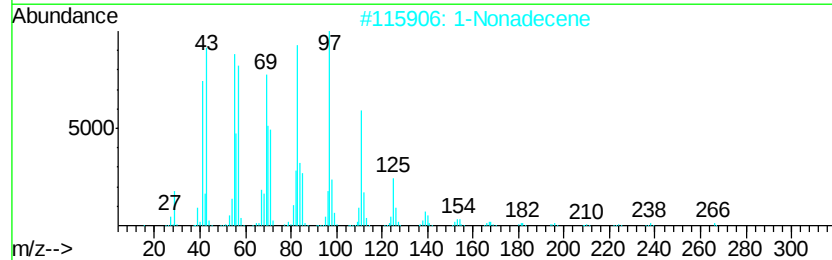
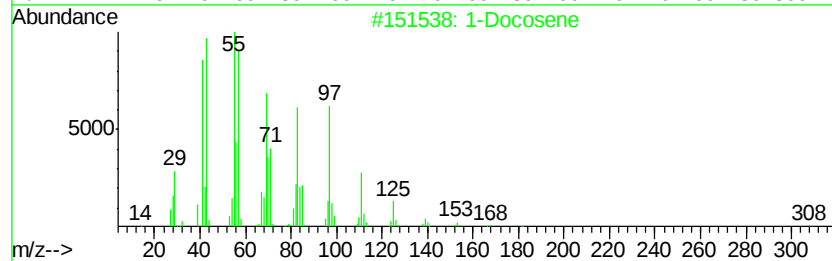
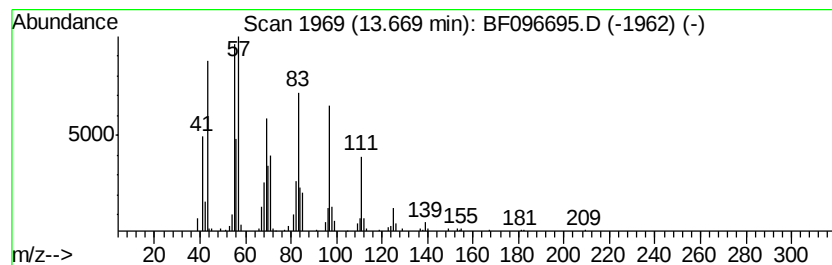
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Peak Number 4 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.67	6.43 ng	181753	Chrysene-d12	13.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	93
2		1-Nonadecene	266	C19H38	018435-45-5	91
3		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
4		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	90
5		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown4.85	4.85	11.8	ng	442938	1	6.67	751231	20.0
unknown6.44	6.44	66.8	ng	2509430	1	6.67	751231	20.0
1-Docosene	13.67	6.4	ng	181753	5	13.80	565683	20.0