

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062216\
 Data File : BF088252.D
 Acq On : 22 Jun 2016 16:25
 Operator : UM/SJ
 Sample : H3660-04
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-2(4-4.5)

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-BF060716.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	1.724	11	12	42	rVB	1292549	2743007	100.00%	15.015%
2	4.730	273	275	288	rBV	236484	371131	13.53%	2.032%
3	5.187	313	315	335	rBV	1441050	1443915	52.64%	7.904%
4	6.261	407	409	411	rBV	1350008	1569680	57.22%	8.592%
5	6.376	417	419	421	rBV	1135374	1565466	57.07%	8.569%
6	6.604	437	439	448	rVB	416237	377616	13.77%	2.067%
7	6.753	450	452	455	rBV	1236752	1174754	42.83%	6.431%
8	7.176	487	489	491	rBV	1034243	995219	36.28%	5.448%
9	7.884	550	551	554	rBV	466795	572979	20.89%	3.136%
10	8.970	643	646	648	rBV	1699993	1750504	63.82%	9.582%
11	9.370	679	681	683	rBV	485325	385896	14.07%	2.112%
12	9.633	702	704	707	rBV	698380	670588	24.45%	3.671%
13	10.422	771	773	776	rBV	1081449	1010352	36.83%	5.531%
14	10.547	782	784	789	rVB	21871	30351	1.11%	0.166%
15	10.993	821	823	825	rBV	27284	29248	1.07%	0.160%
16	11.119	832	834	836	rBV	549290	651104	23.74%	3.564%
17	11.416	859	860	863	rVB	27289	32650	1.19%	0.179%
18	12.696	970	972	974	rBV	1598433	1457429	53.13%	7.978%
19	13.622	1050	1053	1057	rBV2	21143	64151	2.34%	0.351%
20	13.736	1061	1063	1071	rVB	449885	658670	24.01%	3.606%
21	14.811	1154	1157	1159	rBV	19334	27969	1.02%	0.153%
22	15.108	1181	1183	1196	rVB	371814	481746	17.56%	2.637%
23	15.485	1213	1216	1221	rBV	18452	28547	1.04%	0.156%
24	16.845	1331	1335	1338	rBV	71008	132154	4.82%	0.723%
25	17.085	1350	1356	1361	rBV6	9298	43230	1.58%	0.237%

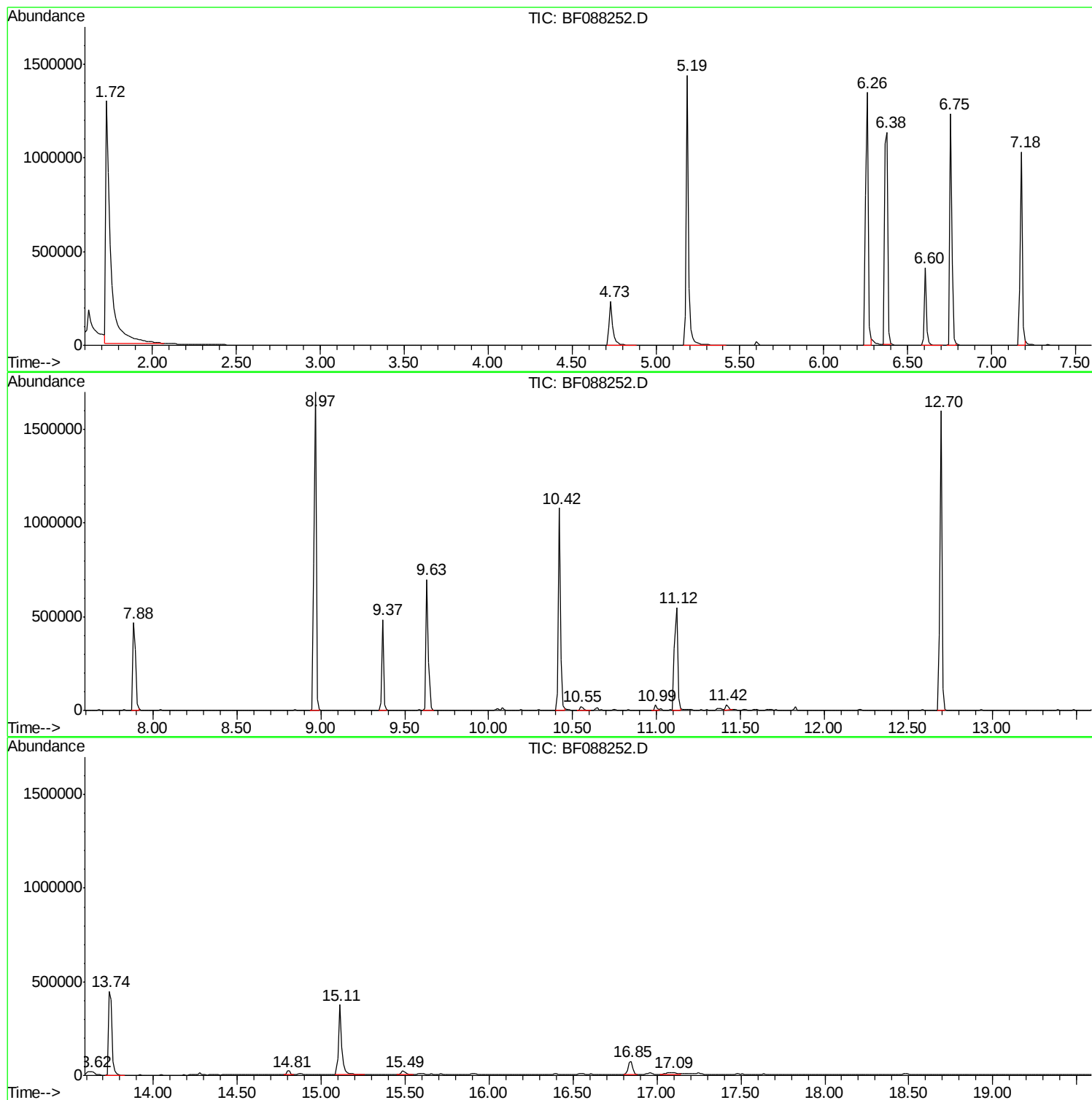
Sum of corrected areas: 18268356

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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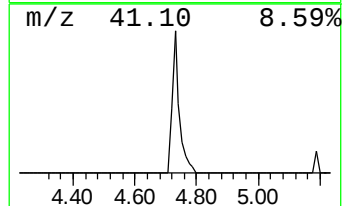
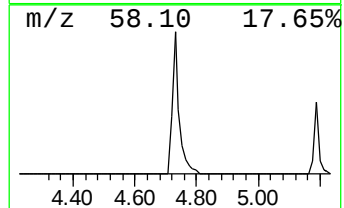
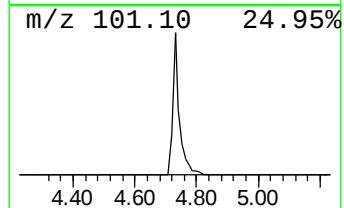
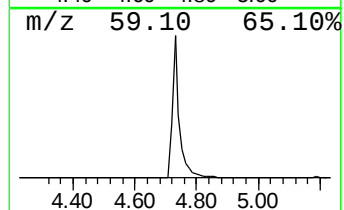
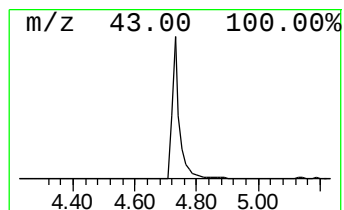
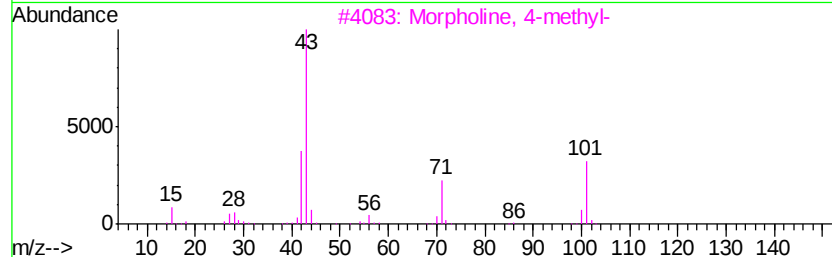
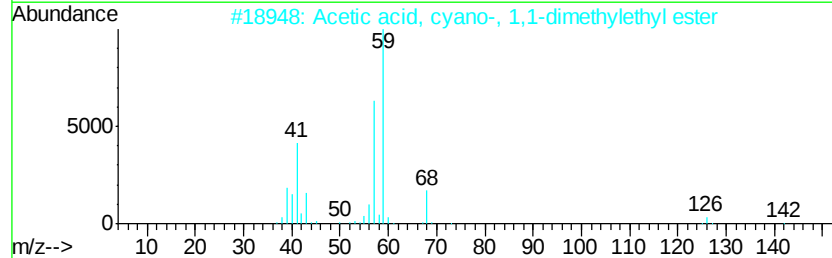
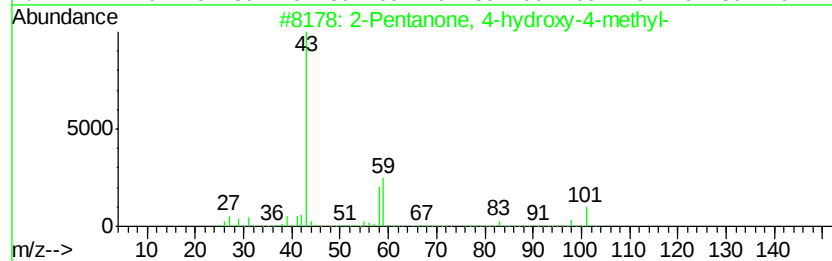
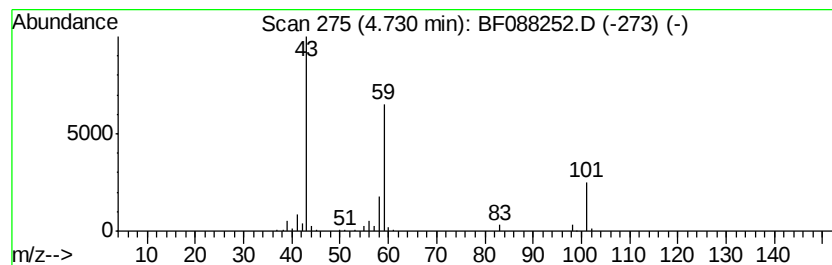
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.73	19.66 ng	371131	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Guanidine	59	CH5N3	000113-00-8	9



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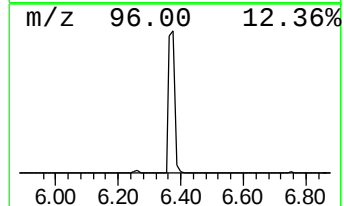
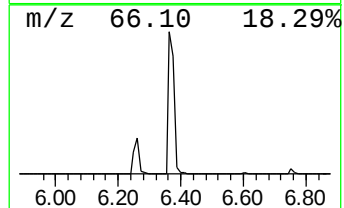
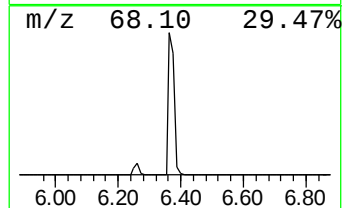
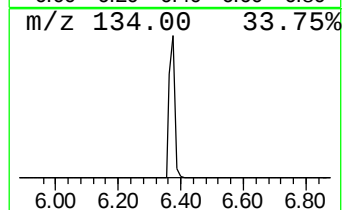
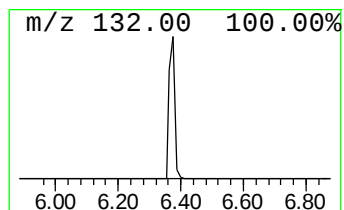
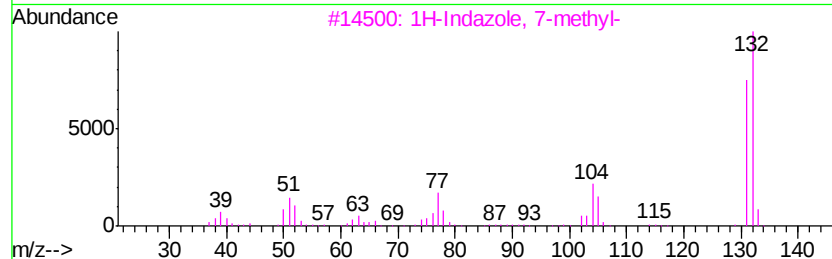
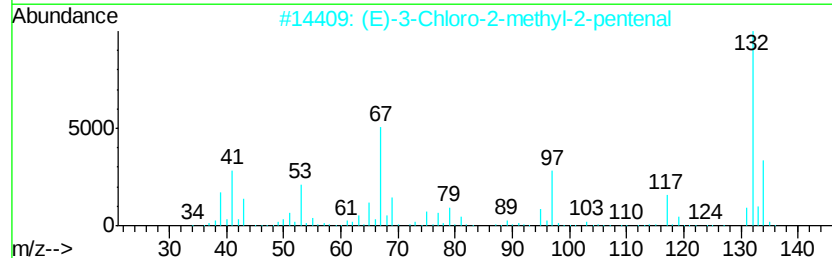
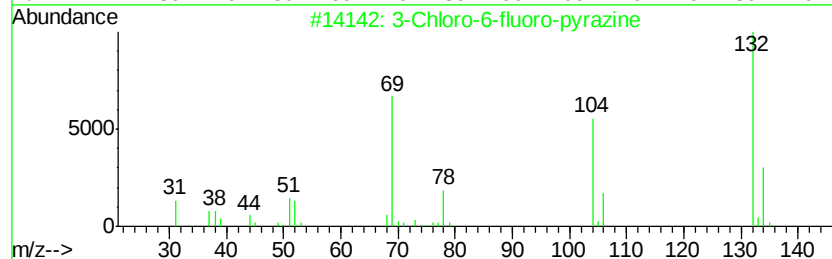
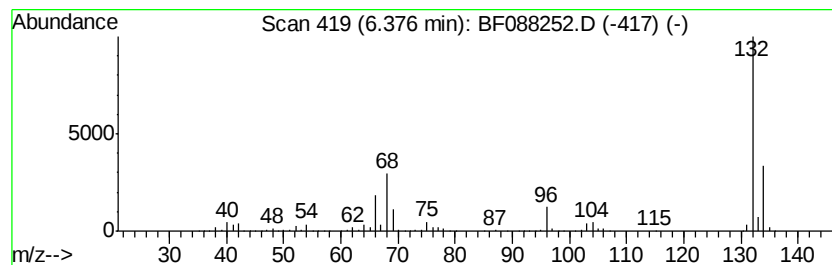
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Peak Number 3 unknown6.38 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.38	82.91 ng	1565470	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	47
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	33
3		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	25
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		Xenon	132	Xe	007440-63-3	9



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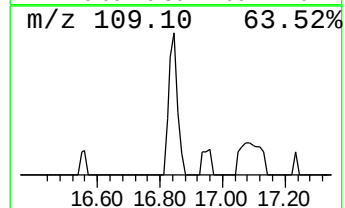
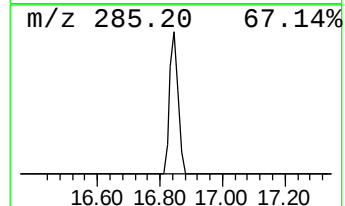
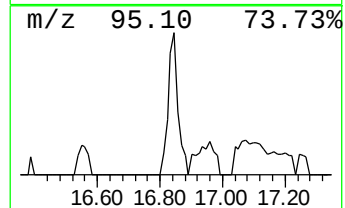
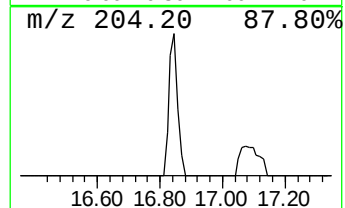
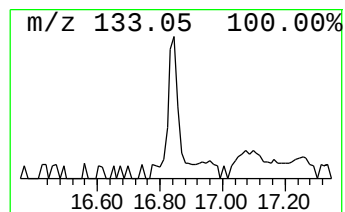
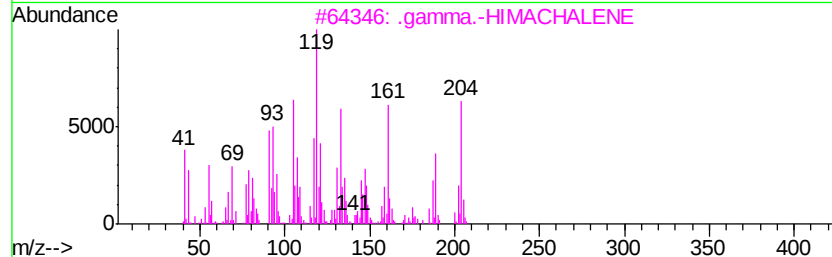
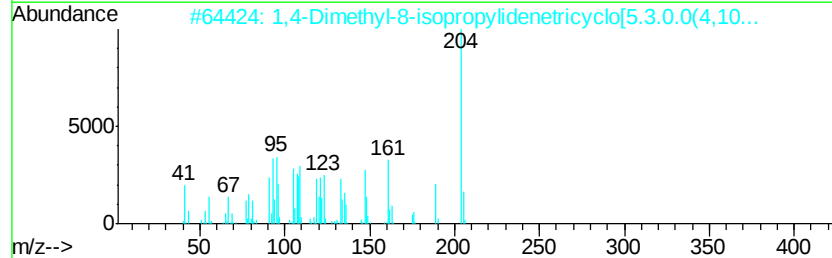
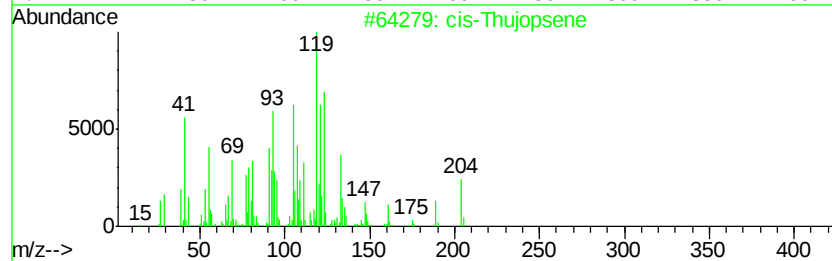
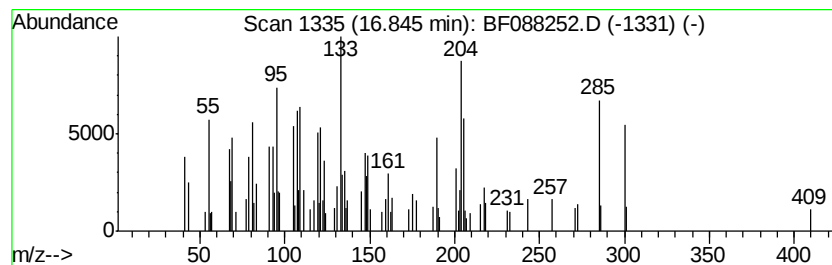
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Peak Number 5 cis-Thujopsene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.85	5.49 ng	132154	Perylene-d12	15.11

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		cis-Thuiopsene	204	C15H24	000470-40-6	64
2		1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	64
3		.gamma.-HIMACHALENE	204	C15H24	1000140-08-0	43
4		1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	38
5		.beta.-l-Galactopyranoside, meth...	394	C16H38O5Si3	056271-59-1	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.73	19.7	ng	371131	1	6.60	377616	20.0
unknown6.38	6.38	82.9	ng	1565470	1	6.60	377616	20.0
cis-Thujopsene	16.85	5.5	ng	132154	6	15.11	481746	20.0