LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
Data File : BF098925.D
Acq On : 28 Sep 2017 23:52
Operator : SJ/JU
Sample : I5472-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-2-3-4-COMP

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-BF092317.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	2.246	22	27	40	rVB	137710	216557	6.36%	0.770%
2	5.151	516	521	533	rVB	585148	771568	22.65%	2.742%
3	5.540	582	587	591	rBV	2981978	3362837	98.73%	11.951%
4	6.545	752	758	767	rVB	3059871	3357152	98.56%	11.931%
5	6.687	777	782	785	rBV	3398099	3406242	100.00%	12.105%
6	6.739	788	791	796	rVB	42099	34713	1.02%	0.123%
7	6.916	817	821	824	rBV	1005301	794991	23.34%	2.825%
8	7.075	843	848	851	rBV	2821042	2592121	76.10%	9.212%
9	7.481	911	917	920	rBV	2014078	2035522	59.76%	7.234%
10	8.198	1035	1039	1042	rBV	1180624	991968	29.12%	3.525%
11	9.275	1216	1222	1225	rBV	3467510	3254853	95.56%	11.567%
12	9.663	1284	1288	1291	rBV	497671	419623	12.32%	1.491%
13	9.951	1333	1337	1341	rBV2	1032269	917621	26.94%	3.261%
14	10.375	1401	1409	1411	rBV	55482	54843	1.61%	0.195%
15	10.739	1467	1471	1475	rBV	1592729	1440744	42.30%	5.120%
16	10.845	1486	1489	1494	rBV	73496	70566	2.07%	0.251%
17	11.439	1586	1590	1593	rBV	892896	714479	20.98%	2.539%
18	13.021	1855	1859	1863	rBV	2334938	2138193	62.77%	7.599%
19	13.904	2006	2009	2018	rBV	127011	142019	4.17%	0.505%
20	14.080	2035	2039	2042	rBV	710746	633531	18.60%	2.251%
21	15.574	2287	2293	2304	rVB	539234	694952	20.40%	2.470%
22	16.027	2367	2370	2374	rVB3	25625	35072	1.03%	0.125%
23	16.551	2455	2459	2469	rVB4	29579	58260	1.71%	0.207%

Sum of corrected areas: 28138427

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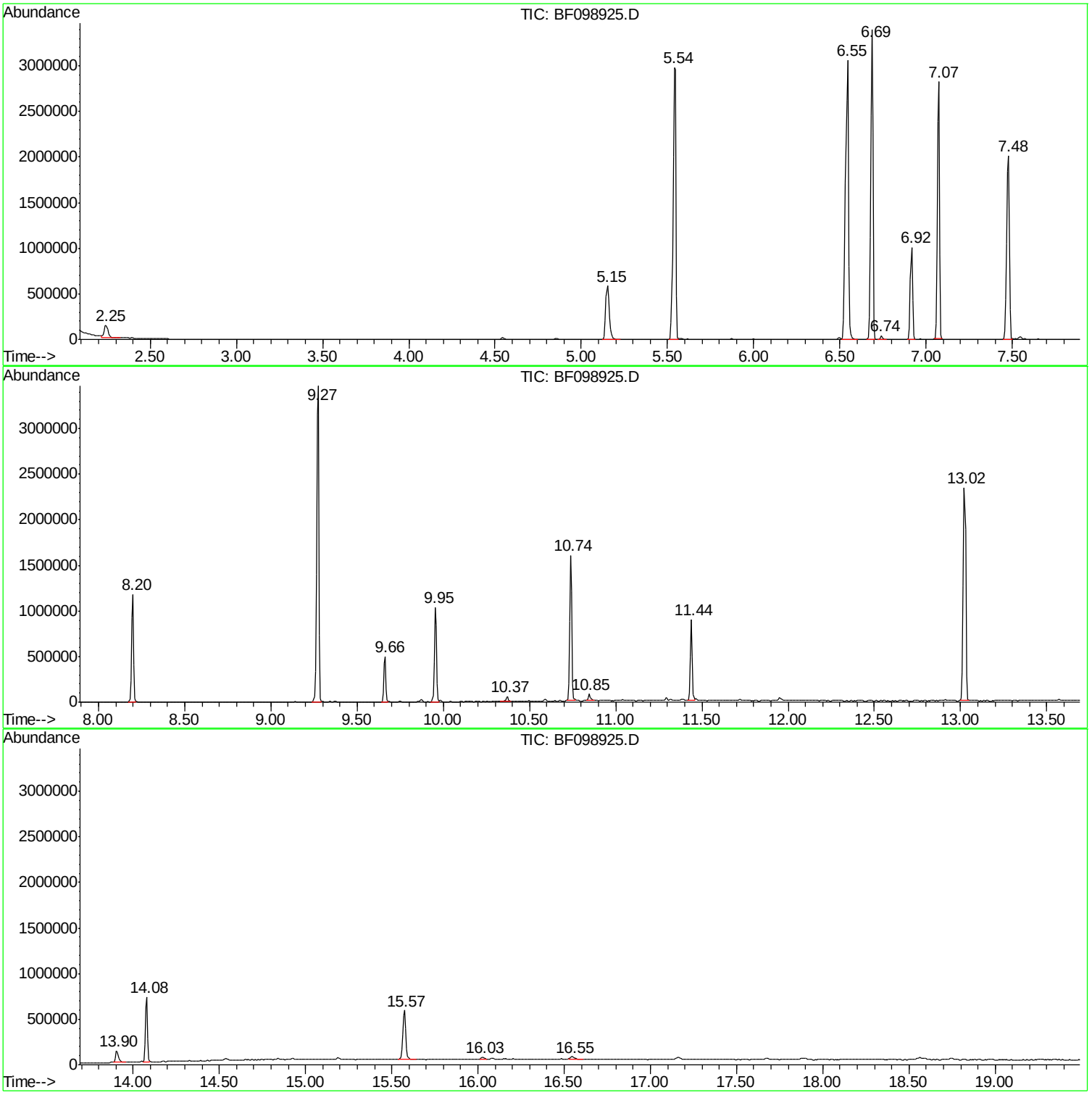
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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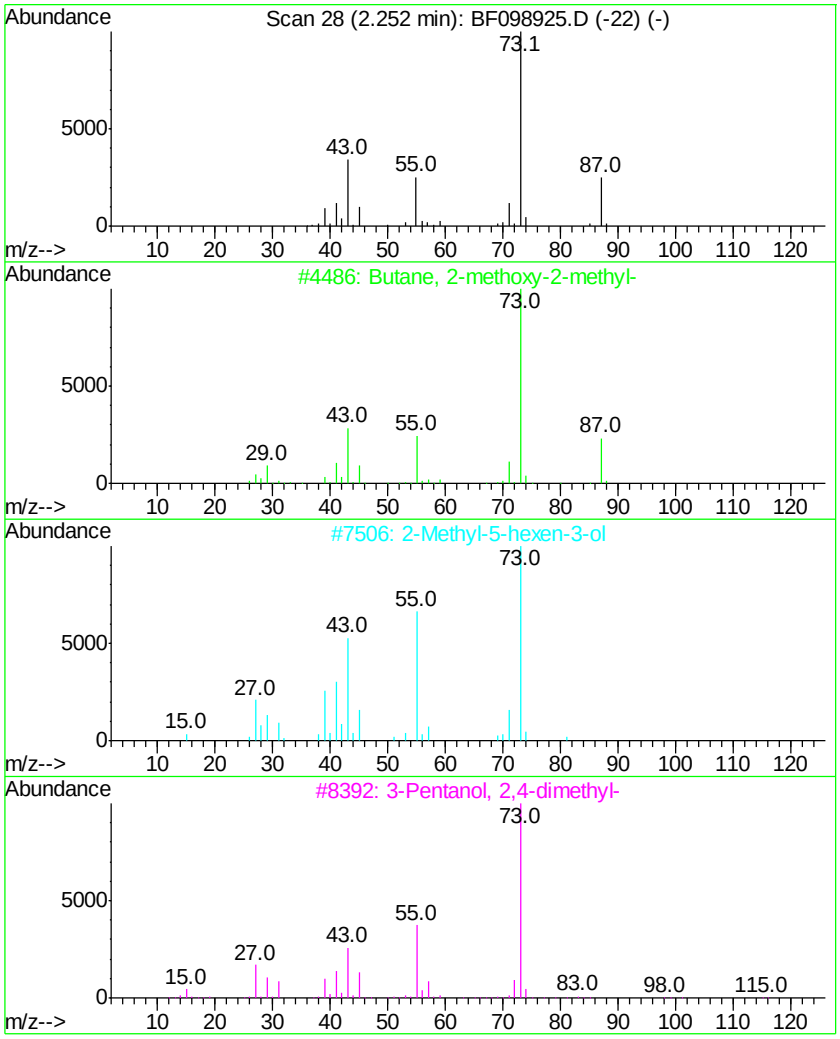
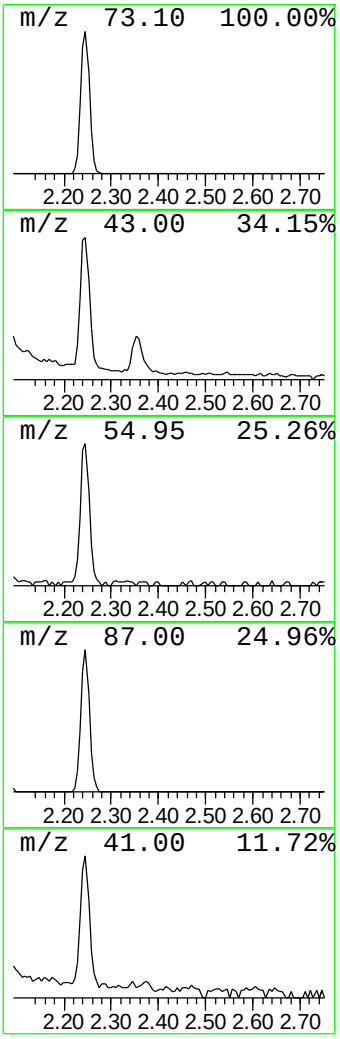
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	5.45 ng	216557	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	40
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	16





Library Search Compound Report

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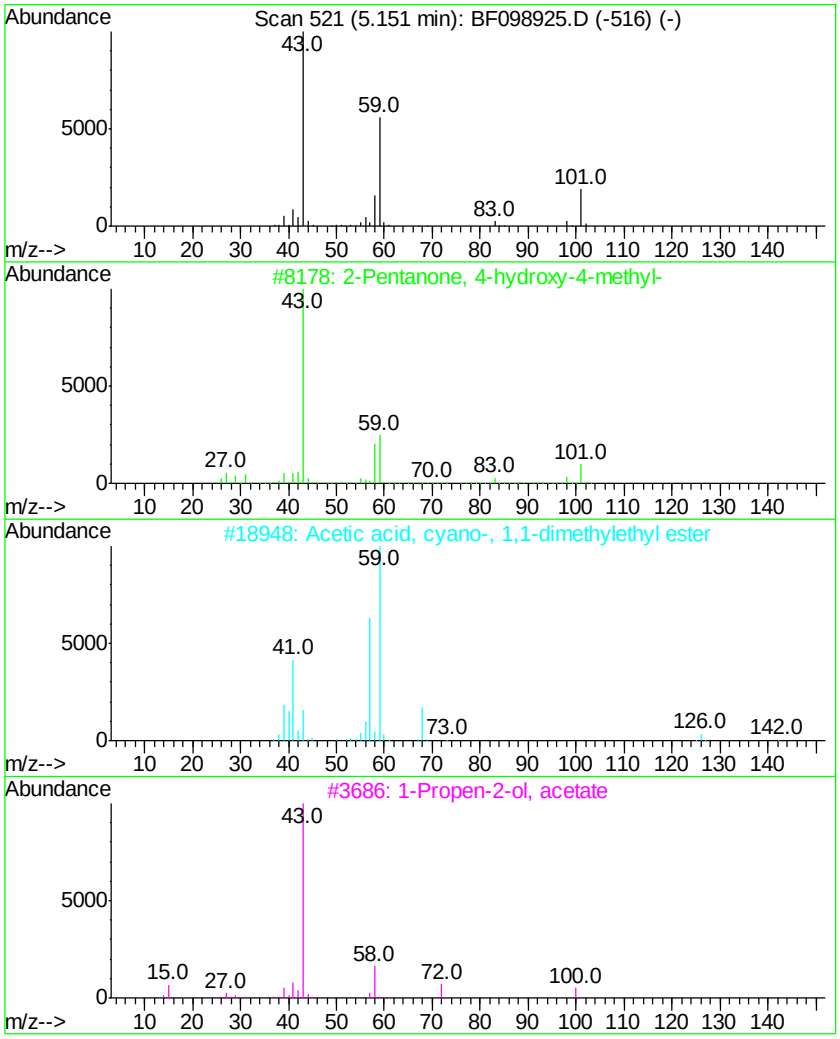
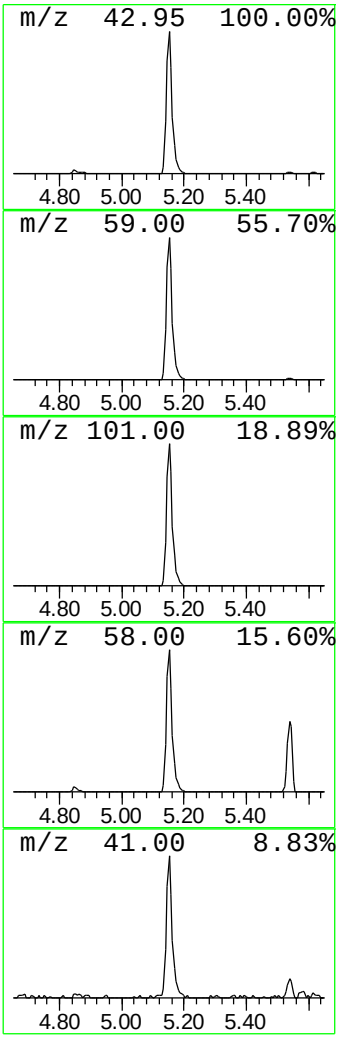
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	19.41 ng	771568	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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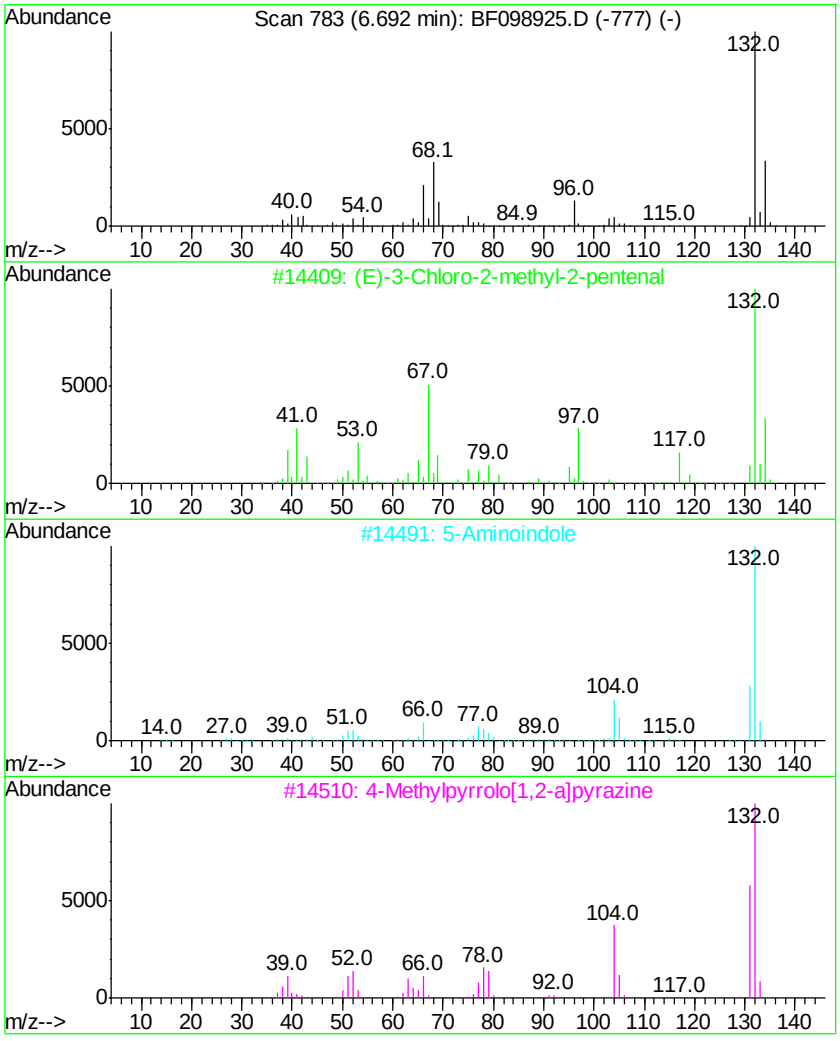
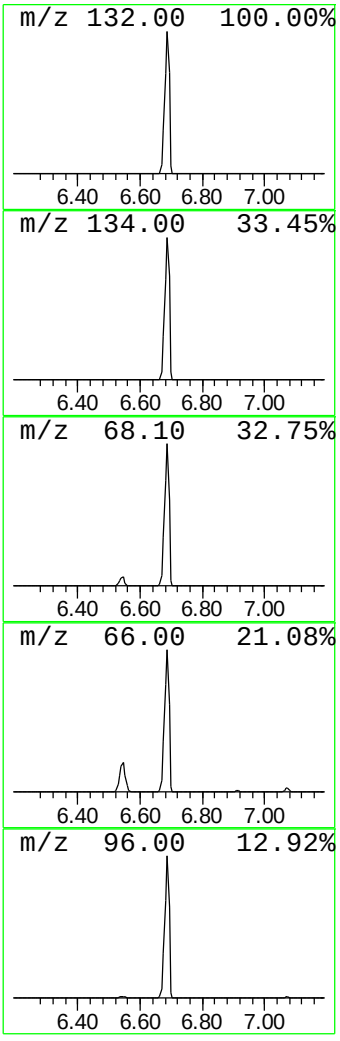
Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	85.69 ng	3406240	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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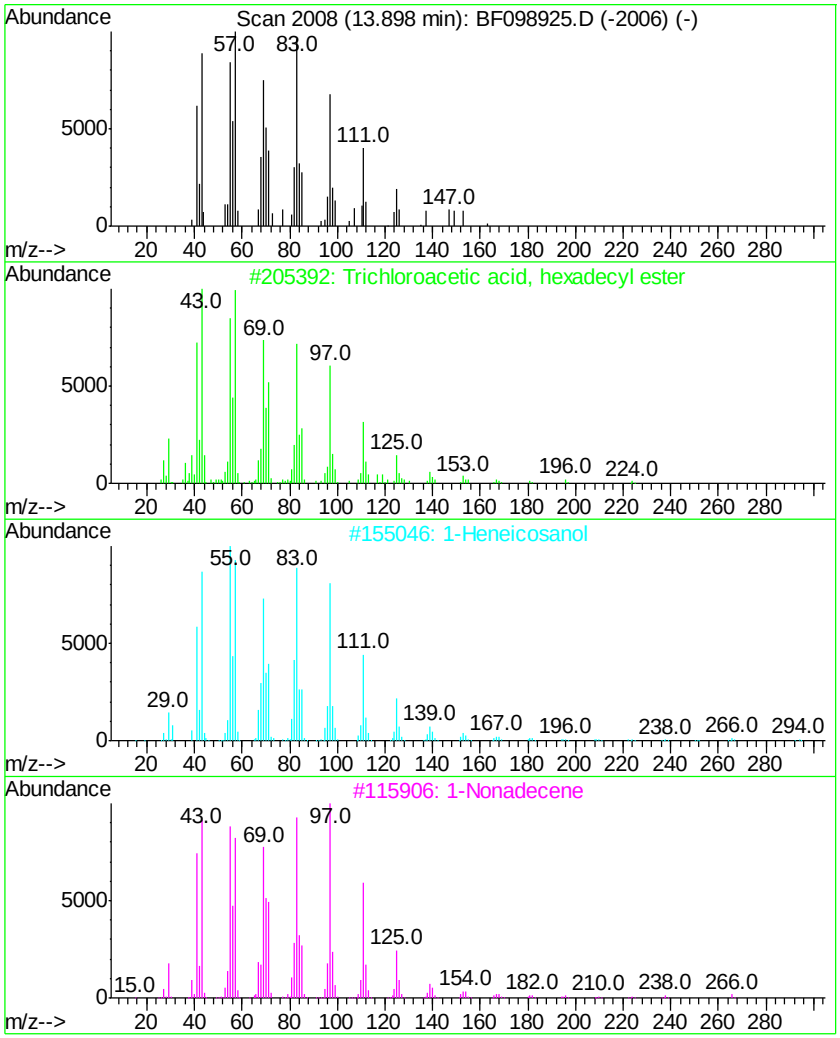
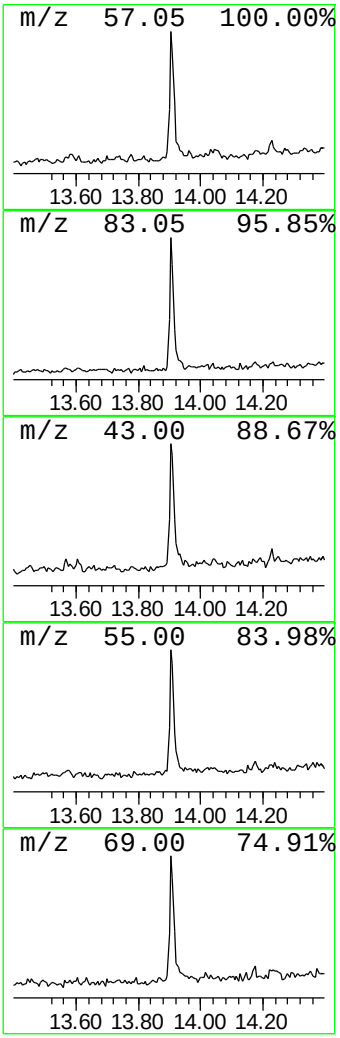
Peak Number 5 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	4.48 ng	142019	Chrysene-d12	14.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	Behenic alcohol	326	C22H46O	000661-19-8	90
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	90





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.25	5.5	ng	216557	1	6.92	794991	20.0
2-Pentanone, 4-hy...	5.15	19.4	ng	771568	1	6.92	794991	20.0
unknown6.69	6.69	85.7	ng	3406240	1	6.92	794991	20.0
Trichloroacetic a...	13.90	4.5	ng	142019	5	14.08	633531	20.0