LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070216\
Data File : BF088622.D
Acq On : 2 Jul 2016 17:38
Operator : UM/SJ
Sample : H3847-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R5-B2(6-12)C

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-BF063016.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	16	rBV	28758	42116	1.76%	0.198%
2	1.850	22	23	34	rVV	129429	258106	10.79%	1.216%
3	1.998	34	36	47	rVB	19015	37414	1.56%	0.176%
4	3.016	123	125	144	rBB	27535	71085	2.97%	0.335%
5	4.284	234	236	239	rBB	26234	32527	1.36%	0.153%
6	4.959	293	295	299	rBV	155445	202610	8.47%	0.955%
7	5.393	330	333	335	rBV	1787340	2391206	100.00%	11.265%
8	6.422	420	423	426	rBV	1694844	2364468	98.88%	11.139%
9	6.559	432	435	437	rBV	2434822	2243338	93.82%	10.568%
10	6.787	453	455	458	rVB	554079	658471	27.54%	3.102%
11	6.947	467	469	472	rVB	1908636	1710649	71.54%	8.059%
12	7.359	502	505	507	rBV	1613775	1645331	68.81%	7.751%
13	8.079	565	568	570	rVB	1111561	926199	38.73%	4.363%
14	9.153	660	662	665	rBV	2265350	2218178	92.76%	10.450%
15	9.553	695	697	699	rBV	366338	393580	16.46%	1.854%
16	9.770	714	716	719	rBV	25105	24310	1.02%	0.115%
17	9.828	719	721	724	rVB	1060257	904082	37.81%	4.259%
18	10.273	759	760	762	rVB	39960	27462	1.15%	0.129%
19	10.616	787	790	792	rBV	1137048	1253227	52.41%	5.904%
20	10.719	797	799	800	rBV	21449	23928	1.00%	0.113%
21	10.742	800	801	806	rVB	42510	44066	1.84%	0.208%
22	11.188	838	840	842	rBV	89661	82829	3.46%	0.390%
23	11.302	848	850	852	rVB	747920	734659	30.72%	3.461%
24	11.371	852	856	858	rBV3	19610	33019	1.38%	0.156%
25	11.611	876	877	880	rBV	38376	50807	2.12%	0.239%
26	11.839	896	897	899	rBV	27245	25090	1.05%	0.118%
27	12.891	986	989	991	rBV	1685128	1483894	62.06%	6.991%
28	13.794	1065	1068	1074	rBV2	70621	103094	4.31%	0.486%
29	13.931	1078	1080	1082	rBV	721374	625036	26.14%	2.945%
30	15.325	1199	1202	1205	rBV	511174	615959	25.76%	2.902%

Sum of corrected areas: 21226740

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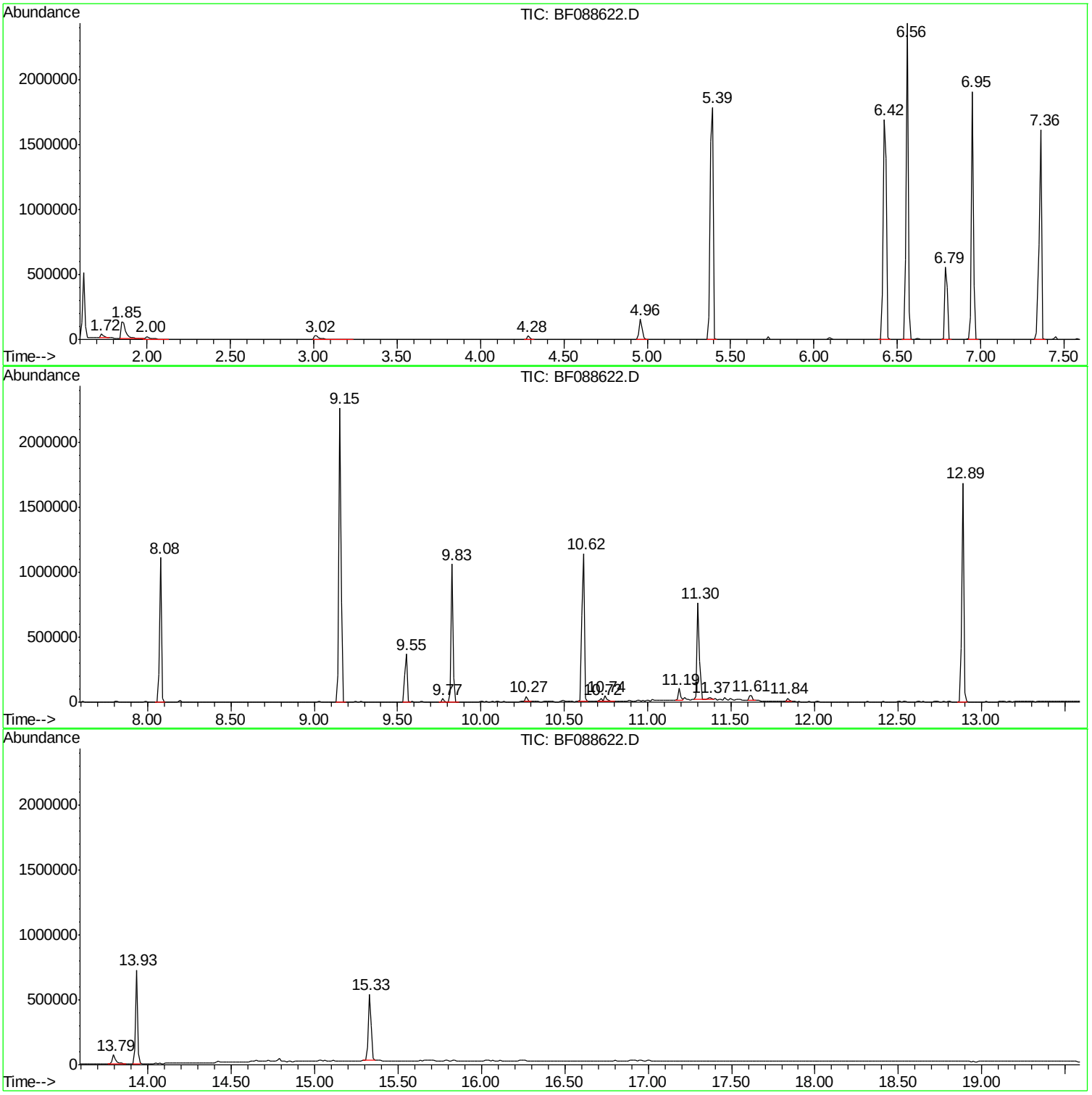
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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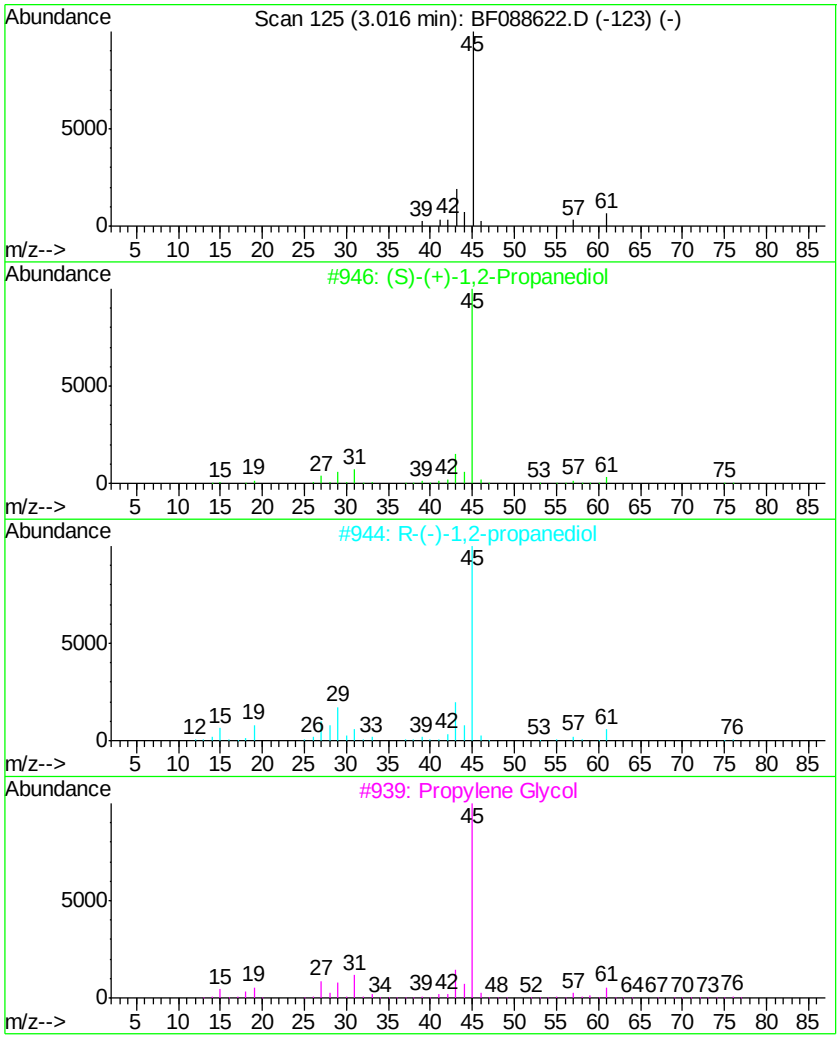
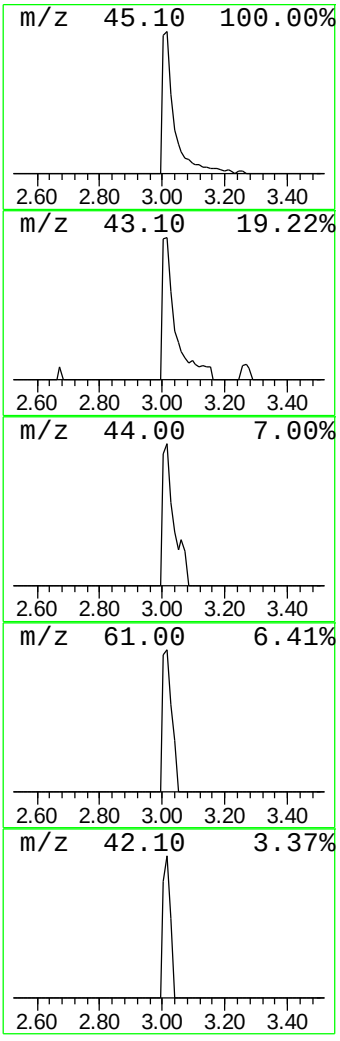
Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.02	2.16 ng	71085	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	74
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	2-Butanol, (R)-	74	C4H10O	014898-79-4	9
5	Formamide	45	CH3NO	000075-12-7	7





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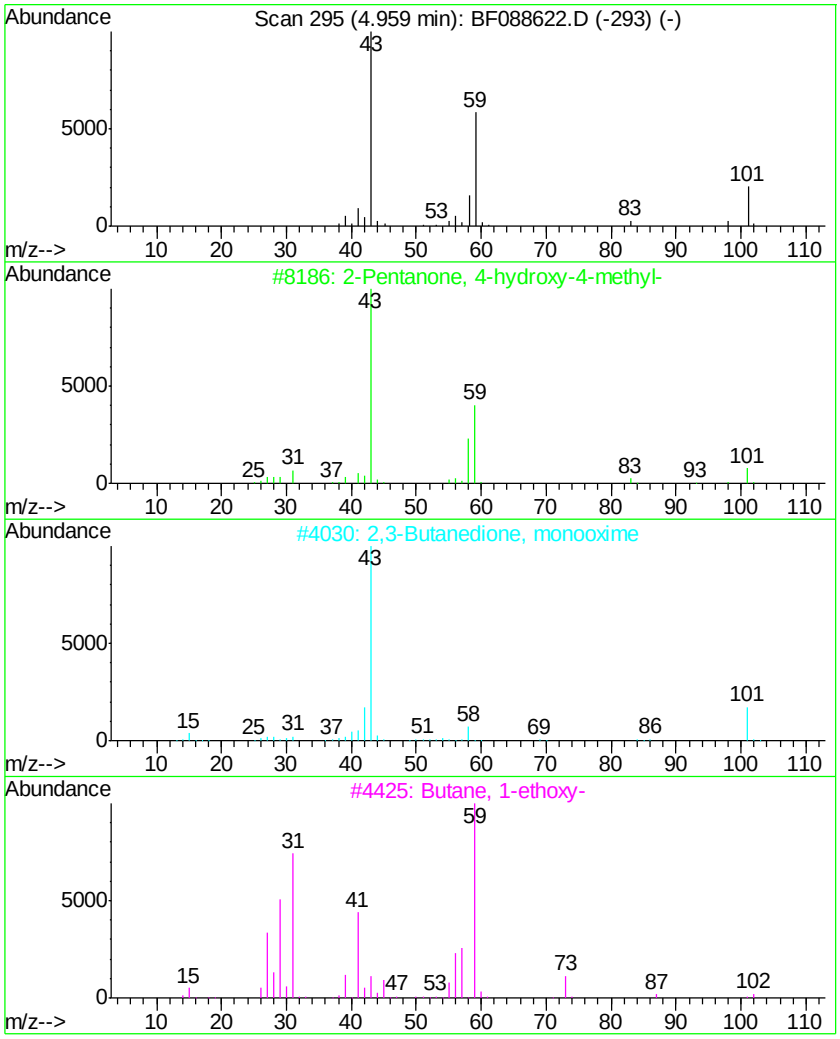
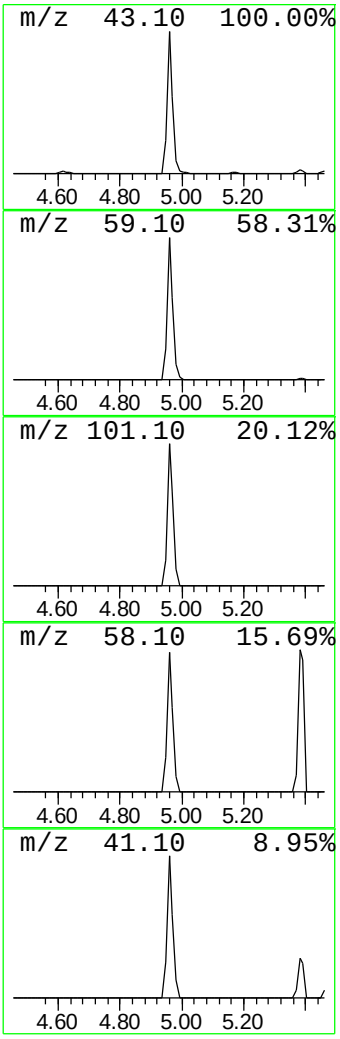
Peak Number 3 unknown4.96 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	6.15 ng	202610	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





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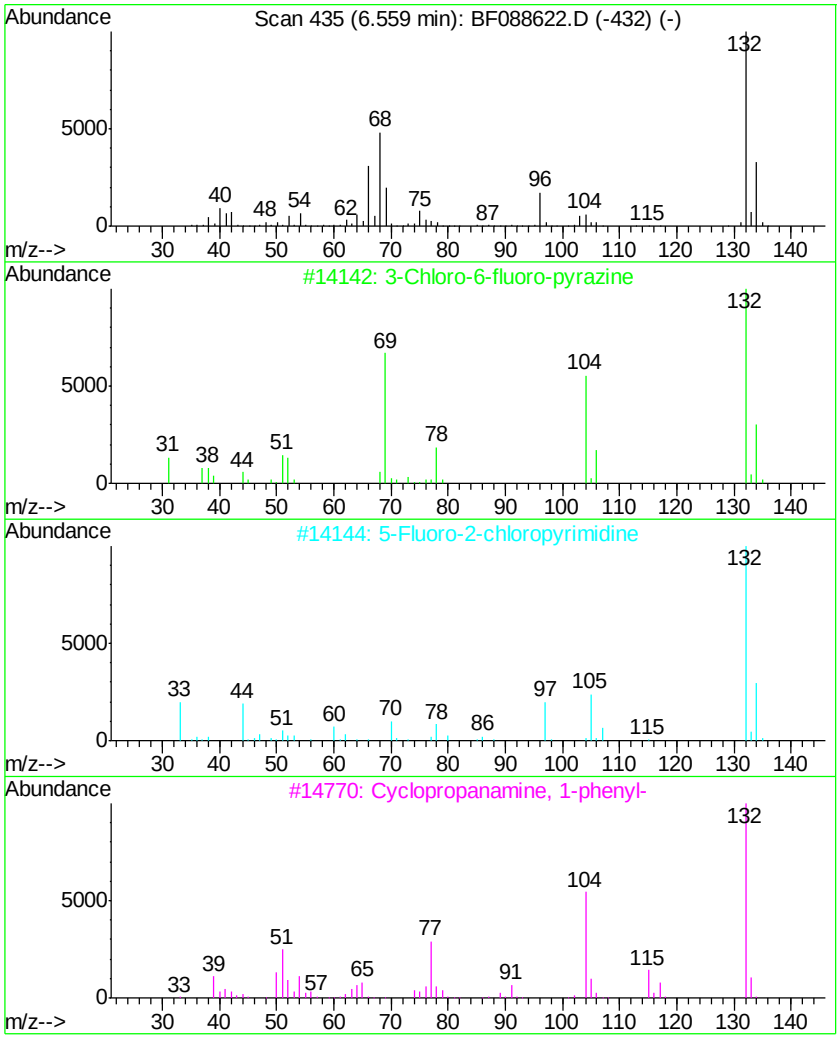
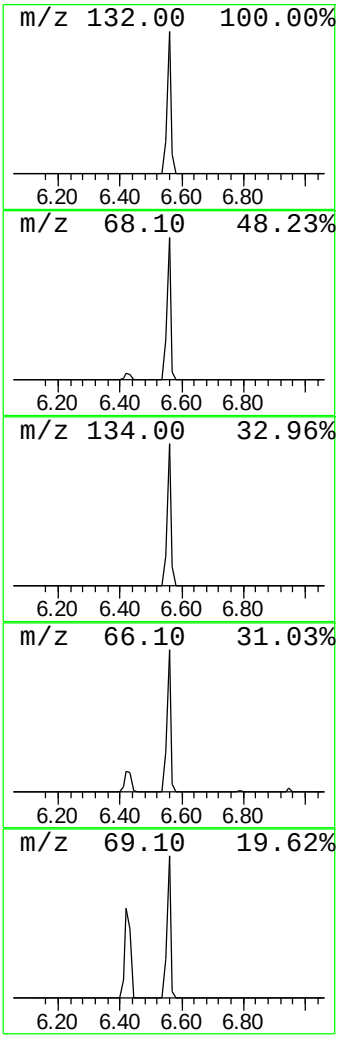
Peak Number 4 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	68.14 ng	2243340	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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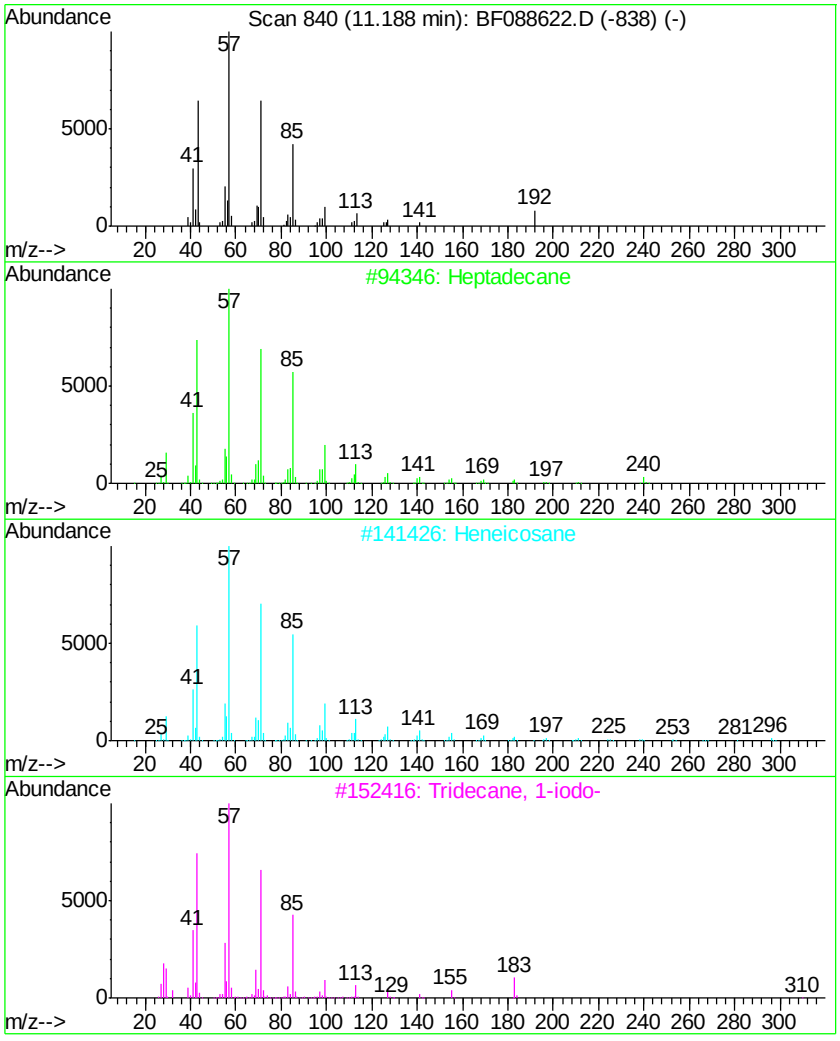
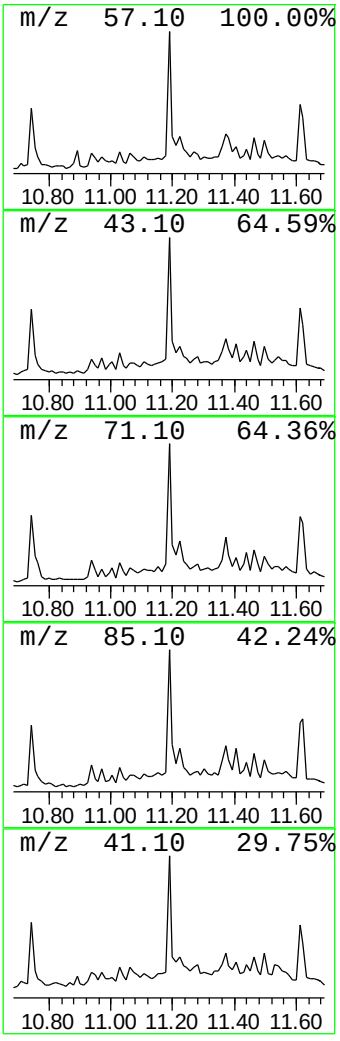
Peak Number 6 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.19	2.25 ng	82829	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Heneicosane	296	C21H44	000629-94-7	90
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87
4	Decane, 2,4,6-trimethyl-	184	C13H28	062108-27-4	86
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80





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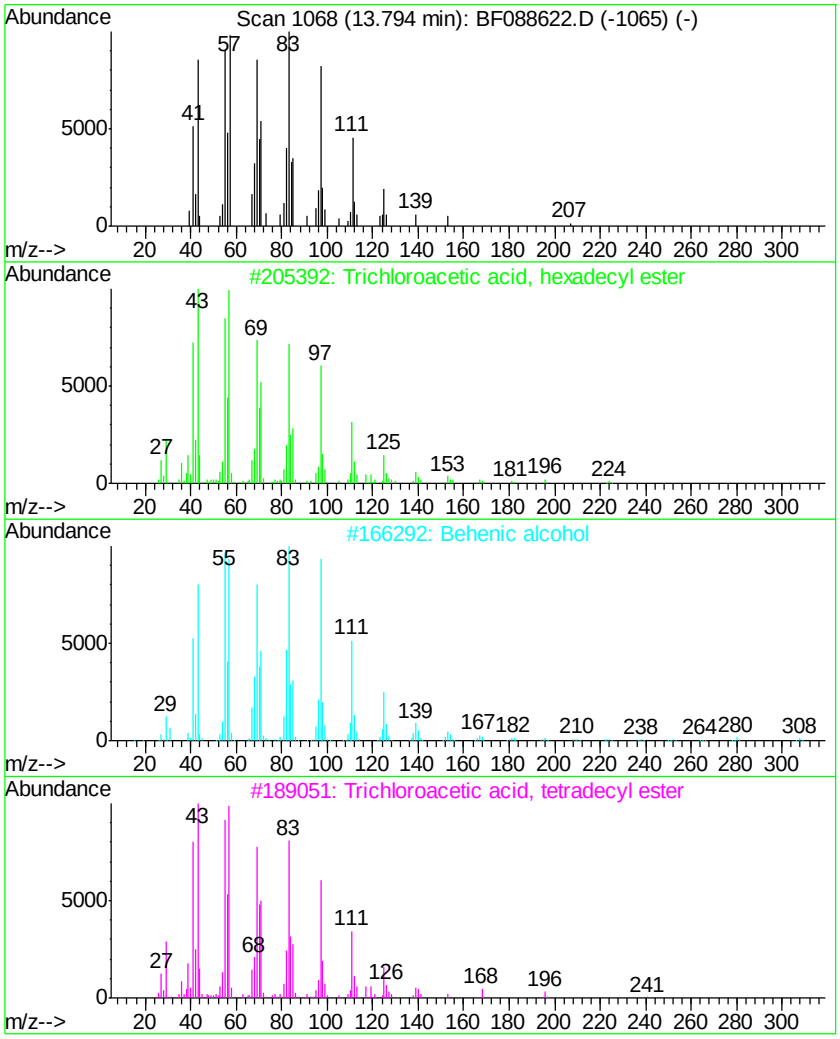
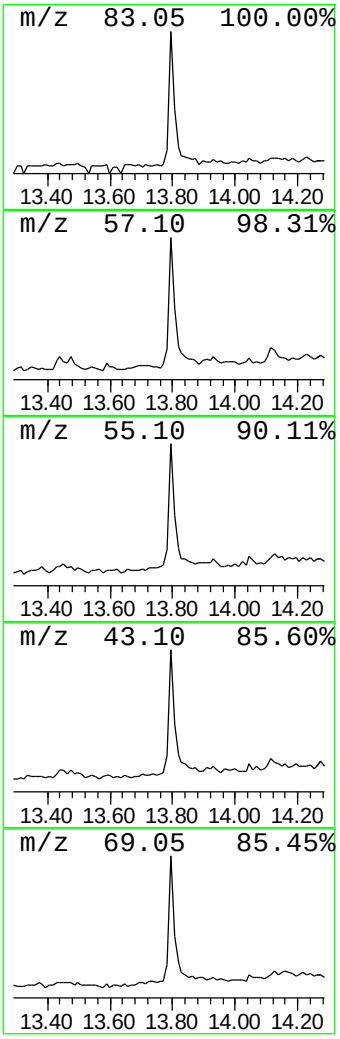
Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	3.30 ng	103094	Chrysene-d12	13.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	91





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(S)-(+)-1,2-Propa...	3.02	2.2	ng	71085	1	6.79	658471	20.0
unknown4.96	4.96	6.2	ng	202610	1	6.79	658471	20.0
unknown6.56	6.56	68.1	ng	2243340	1	6.79	658471	20.0
Heptadecane	11.19	2.3	ng	82829	4	11.30	734659	20.0
Trichloroacetic a...	13.79	3.3	ng	103094	5	13.93	625036	20.0