LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
Data File : BF088630.D
Acq On : 2 Jul 2016 21:32
Operator : UM/SJ
Sample : H3847-17
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R5-B3(0-12)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	1.861	21	24	34	rVB	29803	55631	2.08%	0.263%
2	3.004	123	124	143	rBV2	24955	70731	2.65%	0.335%
3	4.959	293	295	299	rBV	109840	155976	5.84%	0.738%
4	5.393	329	333	335	rBV	1810635	2488000	93.09%	11.772%
5	6.433	421	424	426	rBV	2136176	2672550	100.00%	12.645%
6	6.559	432	435	438	rBV	2390622	2262895	84.67%	10.707%
7	6.787	453	455	458	rVB	487363	657414	24.60%	3.111%
8	6.947	467	469	471	rVB	1827414	1719417	64.34%	8.135%
9	7.359	502	505	507	rBV	1727756	1650559	61.76%	7.810%
10	8.079	566	568	570	rBV	1123270	903129	33.79%	4.273%
11	9.153	660	662	665	rBV	2007963	2259018	84.53%	10.689%
12	9.553	694	697	699	rBV	409234	390093	14.60%	1.846%
13	9.828	719	721	724	rVB	972731	849142	31.77%	4.018%
14	10.273	759	760	762	rVB	44654	31133	1.16%	0.147%
15	10.616	787	790	792	rBV	1254602	1245411	46.60%	5.893%
16	10.742	800	801	805	rVB	45172	48636	1.82%	0.230%
17	11.188	838	840	842	rBV	87169	86025	3.22%	0.407%
18	11.302	848	850	852	rVB2	624721	670859	25.10%	3.174%
19	11.371	852	856	860	rVB4	24729	55360	2.07%	0.262%
20	11.611	876	877	880	rVB	40844	53096	1.99%	0.251%
21	12.891	986	989	991	rBV	1625046	1420729	53.16%	6.722%
22	13.748	1056	1064	1066	rBV5	10378	45920	1.72%	0.217%
23	13.794	1066	1068	1074	rVB2	90664	119263	4.46%	0.564%
24	13.931	1078	1080	1083	rBV	738419	671284	25.12%	3.176%
25	15.325	1200	1202	1205	rBV	365884	552582	20.68%	2.615%

Sum of corrected areas: 21134853

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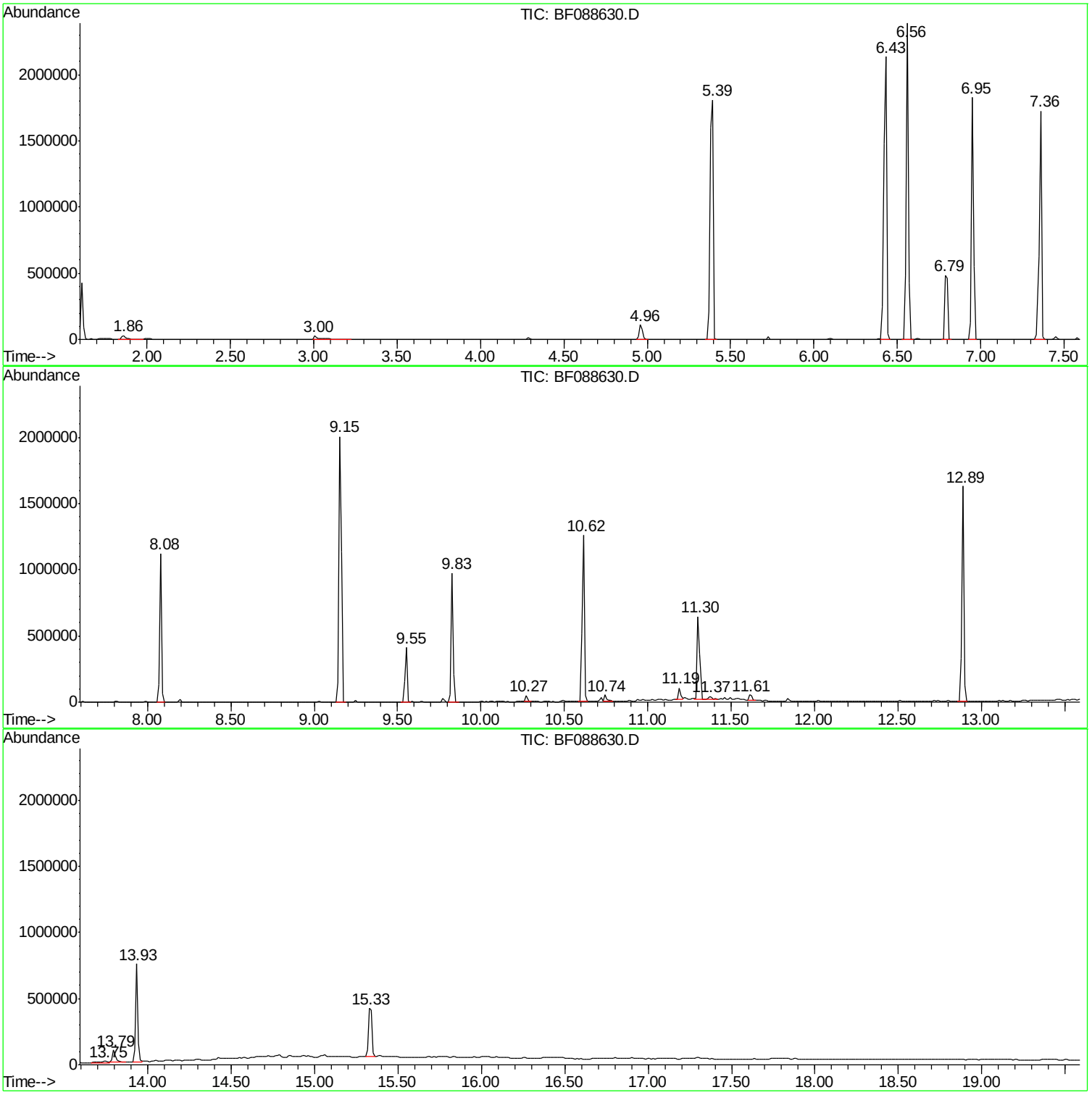
R5-B3(0-12)C

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



Library Search Compound Report

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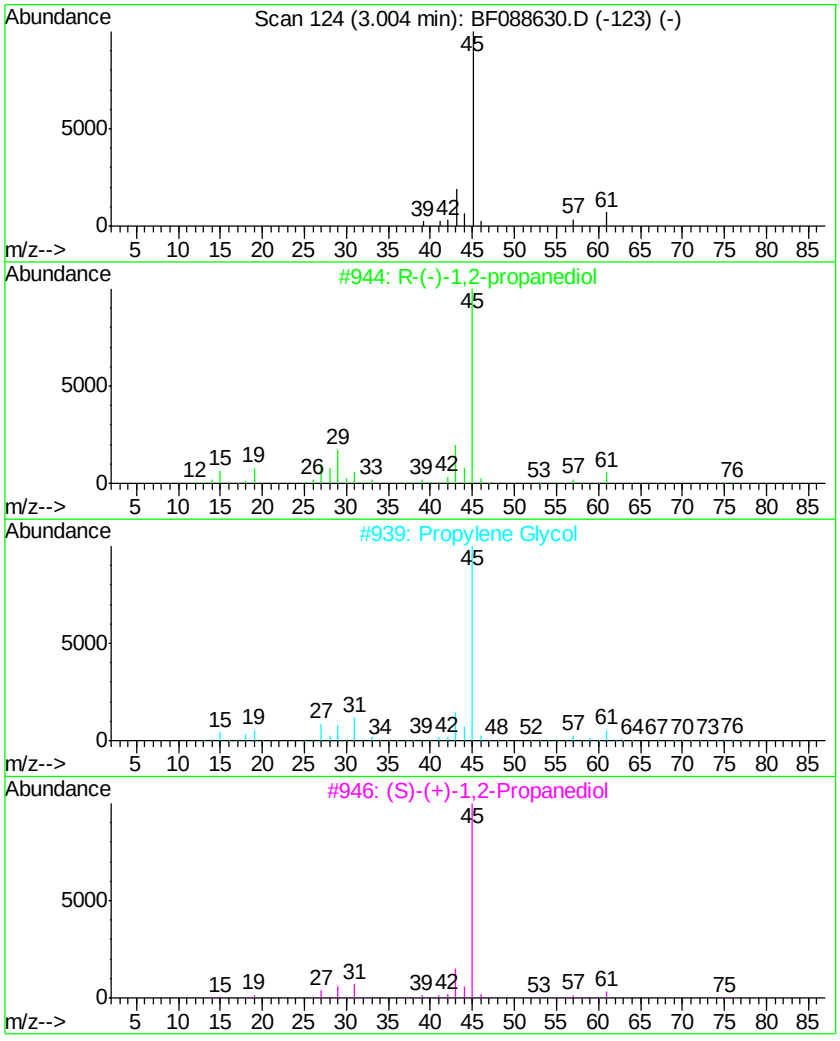
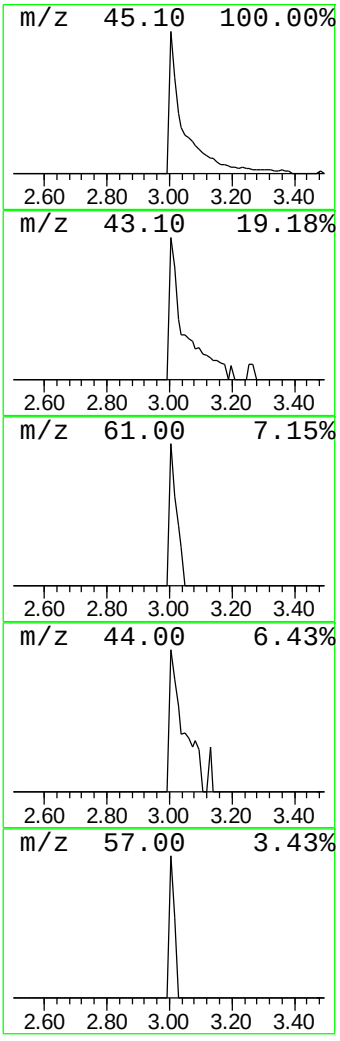
Peak Number 1 R-(-)-1,2-propanediol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.00	2.15 ng	70731	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
2	Propylene Glycol	76	C3H8O2	000057-55-6	9
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
4	Formamide	45	CH3NO	000075-12-7	7
5	2,3-Butanediol	90	C4H10O2	000513-85-9	4





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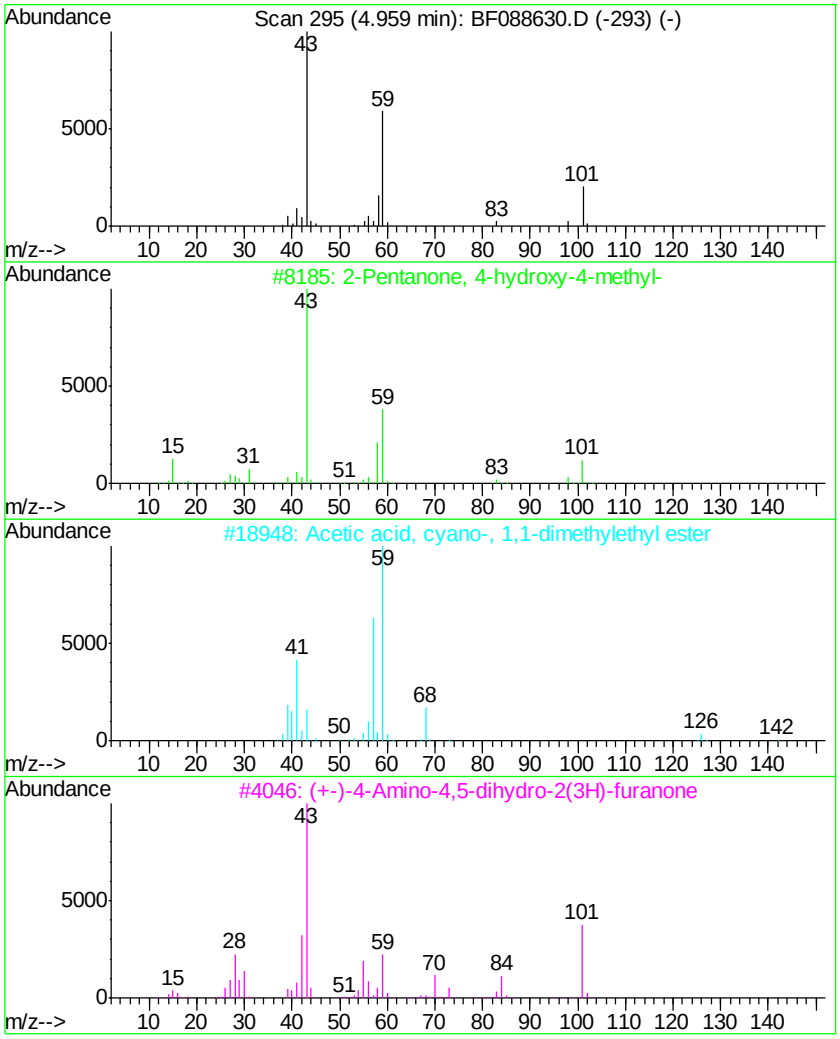
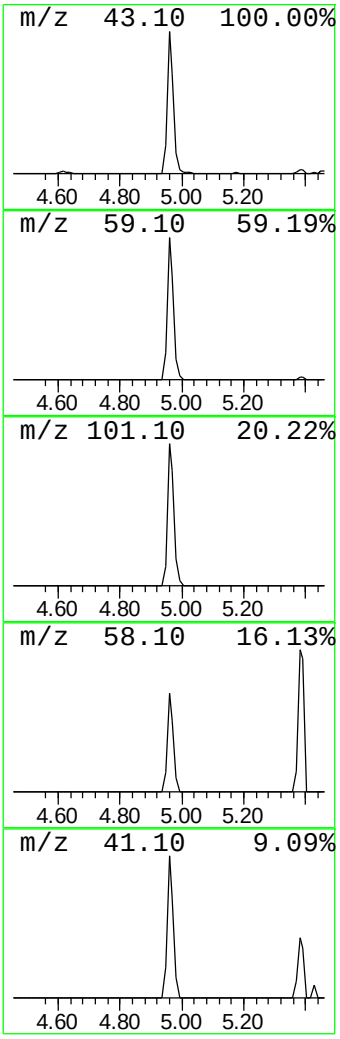
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	4.75 ng	155976	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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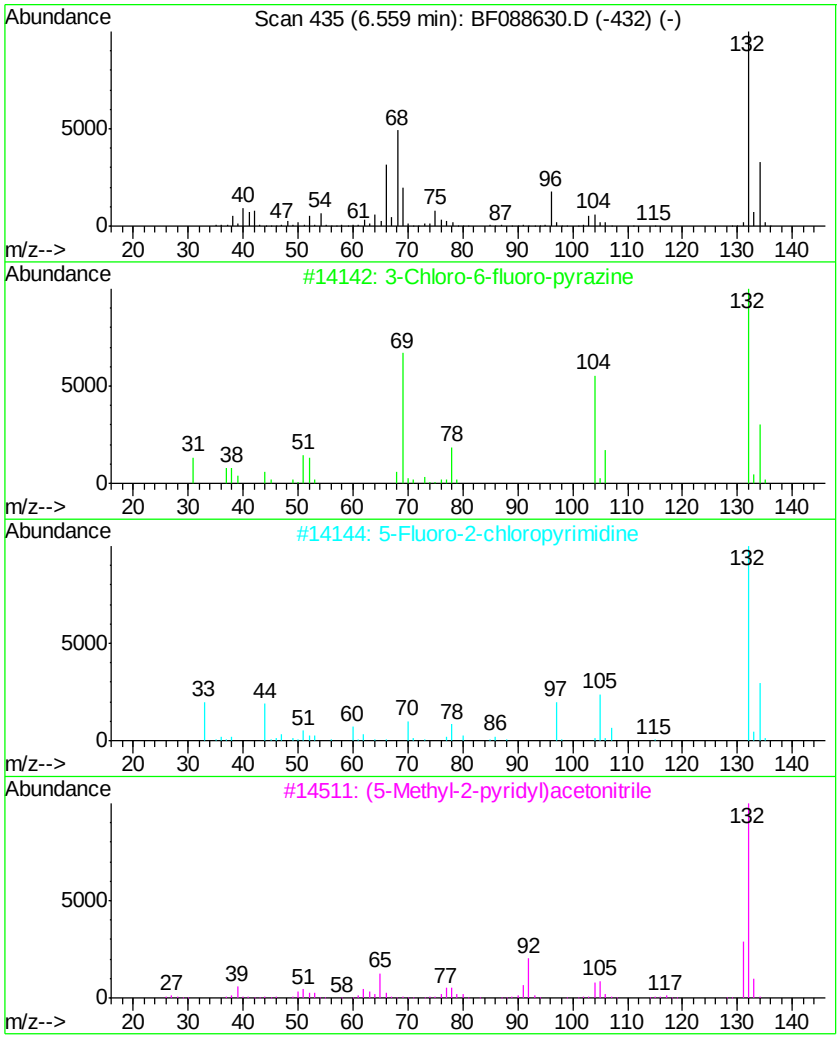
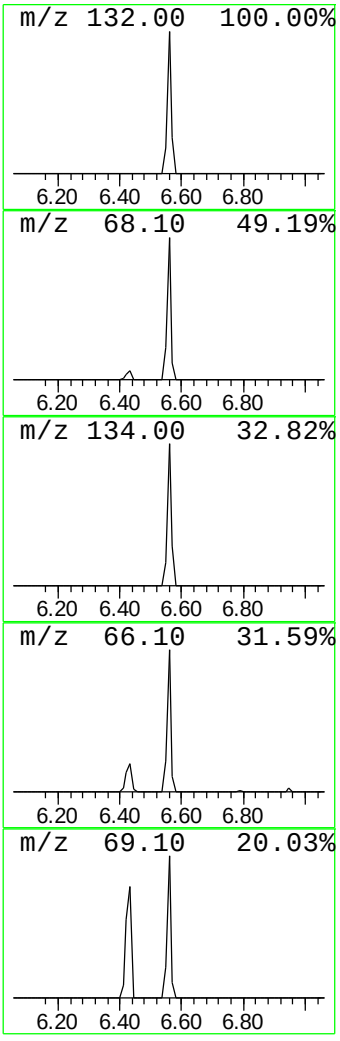
Peak Number 3 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	68.84 ng	2262900	1,4-Dichlorobenzene-d4	6.80

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	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





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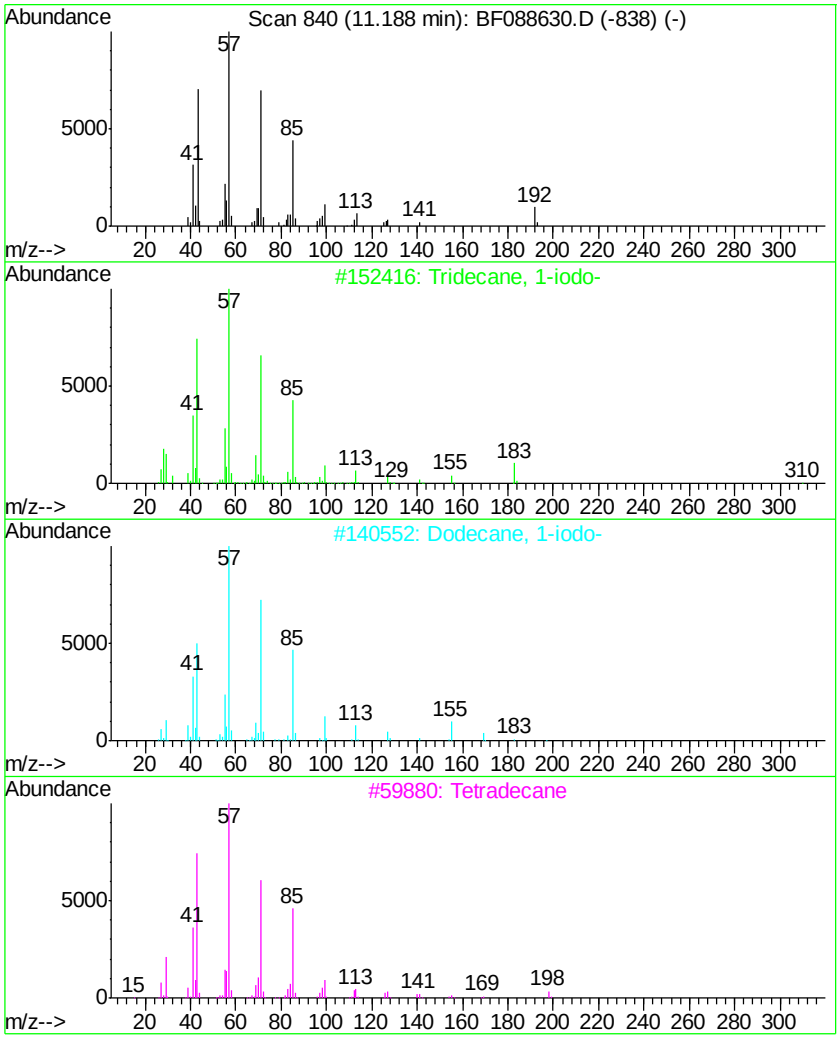
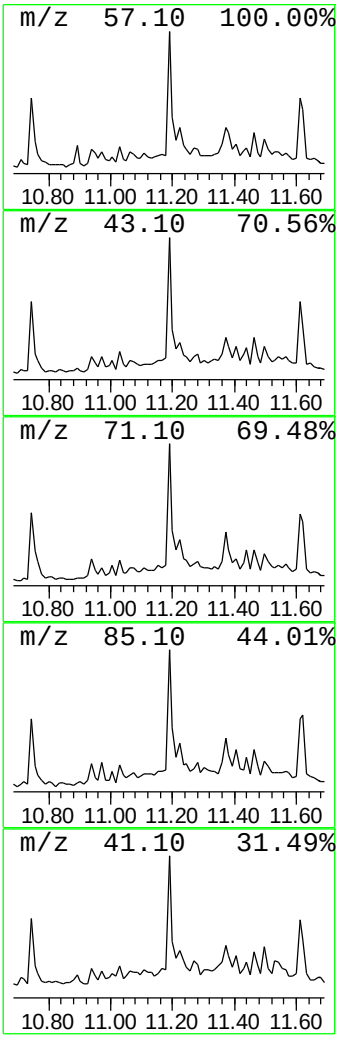
Peak Number 5 Tridecane, 1-iodo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.19	2.56 ng	86025	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
2	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
3	Tetradecane	198	C14H30	000629-59-4	80
4	Hexadecane	226	C16H34	000544-76-3	72
5	Tridecane, 7-propyl-	226	C16H34	055045-09-5	72





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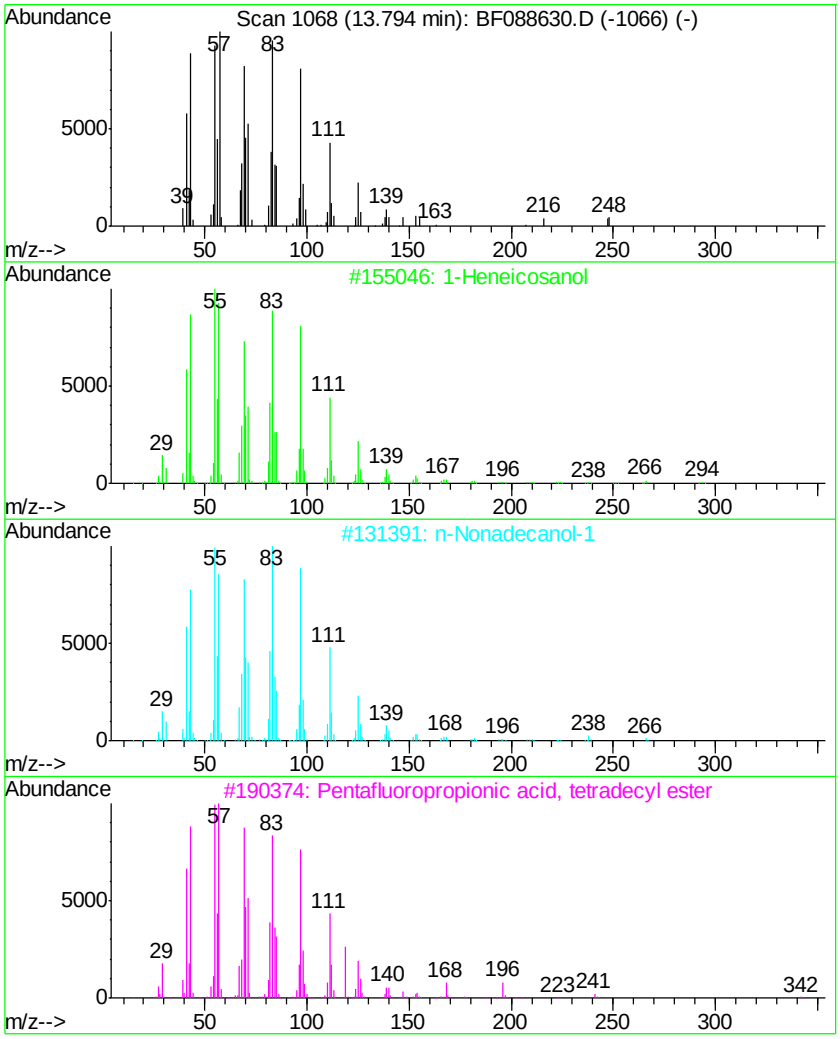
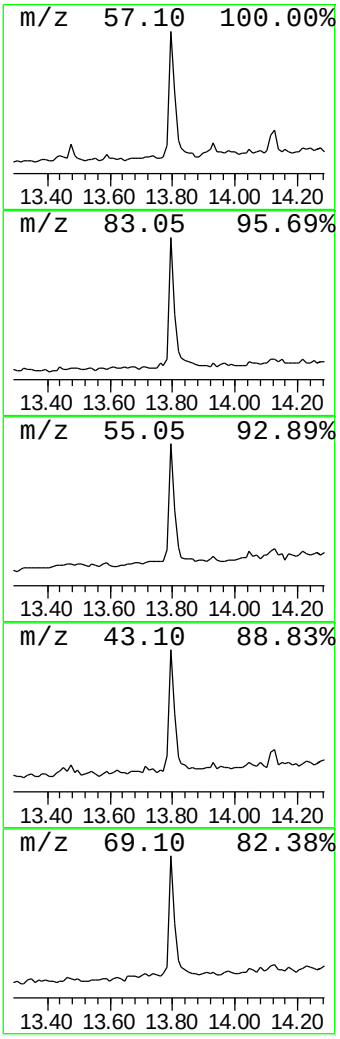
Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	3.55 ng	119263	Chrysene-d12	13.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
R-(-)-1,2-propane...	3.00	2.1	ng	70731	1	6.80	657414	20.0
2-Pentanone, 4-hy...	4.96	4.8	ng	155976	1	6.80	657414	20.0
unknown6.56	6.56	68.8	ng	2262900	1	6.80	657414	20.0
Tridecane, 1-iodo-	11.19	2.6	ng	86025	4	11.30	670859	20.0
1-Heneicosanol	13.79	3.5	ng	119263	5	13.93	671284	20.0