LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071917\
Data File : BF096877.D
Acq On : 19 Jul 2017 18:35
Operator : SJ/JU
Sample : I4243-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-CN

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-BF071317.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	2.834	142	144	157	rBV	75975	146599	6.06%	0.653%
2	4.757	468	471	481	rVB	171504	243944	10.08%	1.086%
3	5.198	541	546	549	rBV	2219479	2419289	100.00%	10.775%
4	6.239	717	723	733	rBV	2209473	2343966	96.89%	10.440%
5	6.357	738	743	746	rBV	2367426	2221150	91.81%	9.893%
6	6.587	778	782	788	rBV	680989	582331	24.07%	2.594%
7	6.745	804	809	812	rBV	1716647	1686419	69.71%	7.511%
8	7.151	873	878	881	rBV	1436802	1395505	57.68%	6.215%
9	7.275	892	899	905	rVB	40232	56202	2.32%	0.250%
10	7.869	995	1000	1003	rBV	903500	791273	32.71%	3.524%
11	8.945	1178	1183	1187	rBV	2343700	2414756	99.81%	10.755%
12	9.345	1246	1251	1254	rBV	576174	511885	21.16%	2.280%
13	9.616	1292	1297	1301	rBV	953958	832872	34.43%	3.710%
14	10.069	1371	1374	1377	rVB	43314	35487	1.47%	0.158%
15	10.404	1426	1431	1434	rBV	1533772	1486506	61.44%	6.621%
16	10.539	1451	1454	1462	rBV	72389	77681	3.21%	0.346%
17	10.986	1523	1530	1532	rBV2	49415	44100	1.82%	0.196%
18	11.092	1543	1548	1551	rBV	1063827	885822	36.61%	3.945%
19	11.339	1584	1590	1596	rVB2	53967	61232	2.53%	0.273%
20	11.410	1598	1602	1605	rBV	28403	26010	1.08%	0.116%
21	11.639	1639	1641	1644	rBV2	35628	34379	1.42%	0.153%
22	12.521	1786	1791	1795	rBV3	28485	37717	1.56%	0.168%
23	12.680	1812	1818	1821	rBV	2286763	2286149	94.50%	10.182%
24	13.168	1894	1901	1907	rBV	291625	300100	12.40%	1.337%
25	13.586	1967	1972	1978	rBV2	134573	154263	6.38%	0.687%
26	13.715	1990	1994	1998	rBV	718609	723107	29.89%	3.221%
27	14.568	2136	2139	2142	rBV2	20518	24330	1.01%	0.108%
28	14.710	2160	2163	2171	rBV3	18926	40919	1.69%	0.182%
29	15.033	2214	2218	2221	rBV	20910	30066	1.24%	0.134%
30	15.086	2223	2227	2232	rVV	473758	558239	23.07%	2.486%

Sum of corrected areas: 22452298

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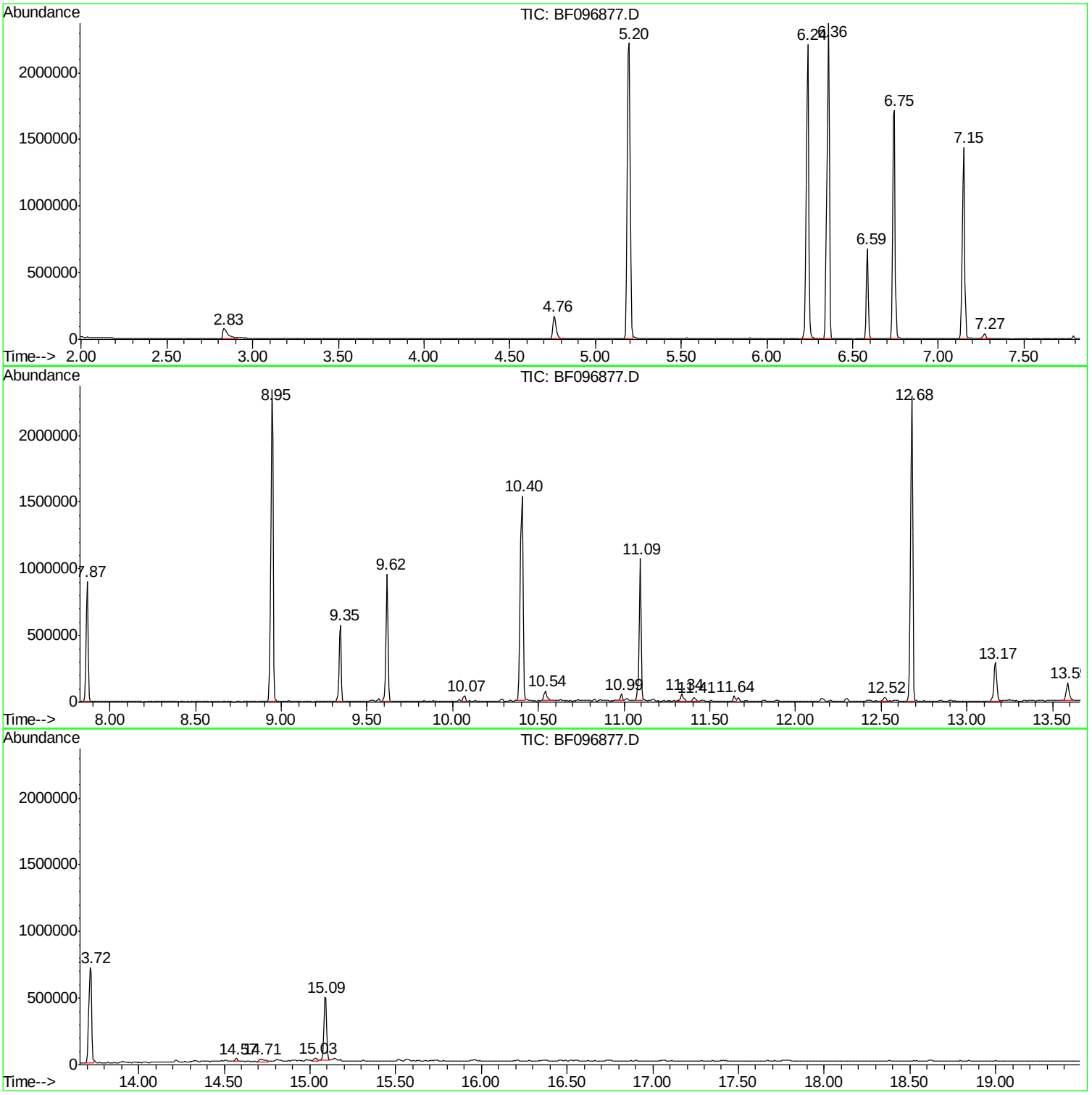
Instrument : BNA_F
ClientSampleId : TP-CN

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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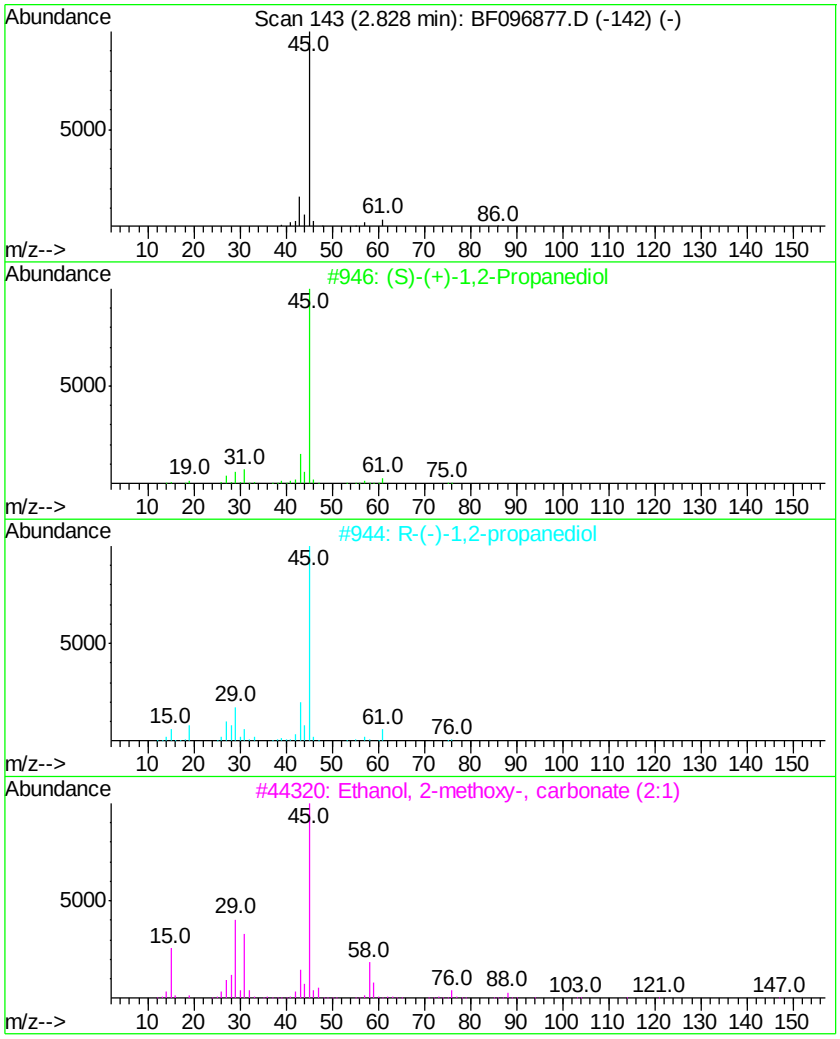
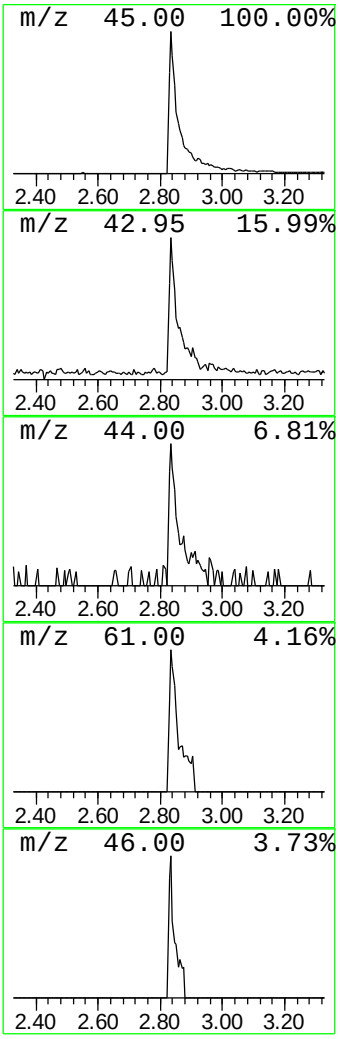
Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.83	5.03 ng	146599	1,4-Dichlorobenzene-d4	6.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
3	Ethanol, 2-methoxy-, carbonate (...	178	C7H14O5	000626-84-6	9
4	Propylene Glycol	76	C3H8O2	000057-55-6	9
5	2-Butanol, (R)-	74	C4H10O	014898-79-4	9





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : TP-CN

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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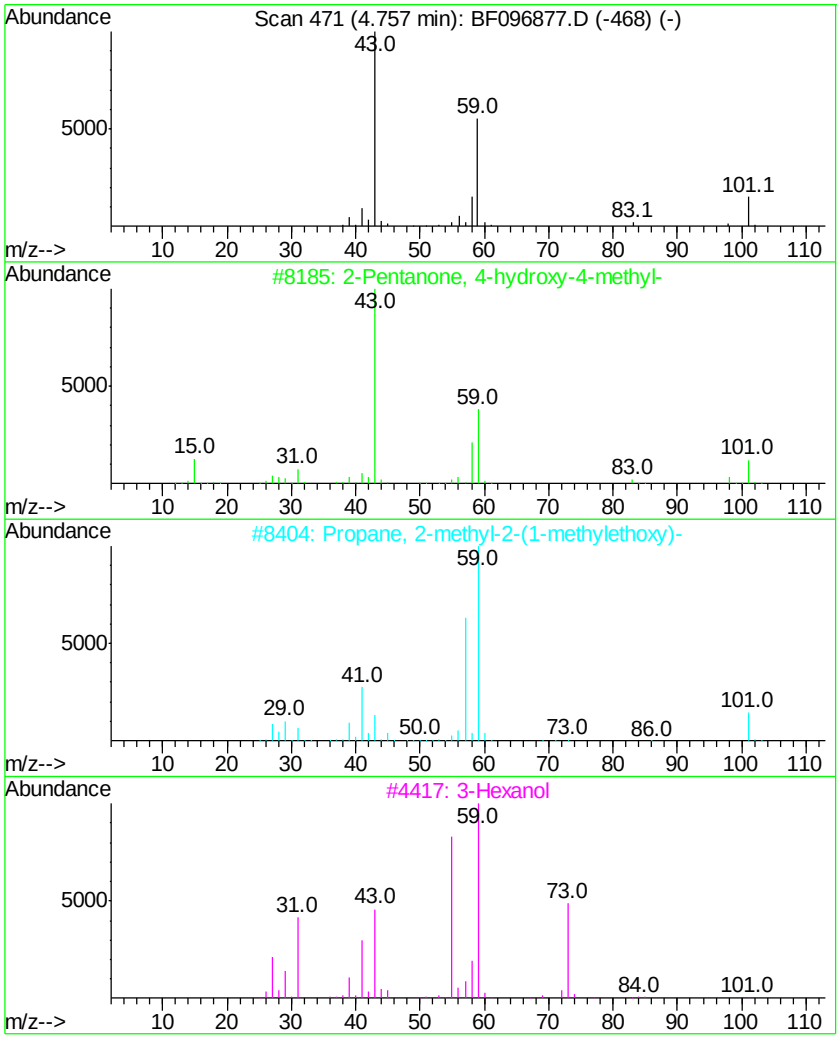
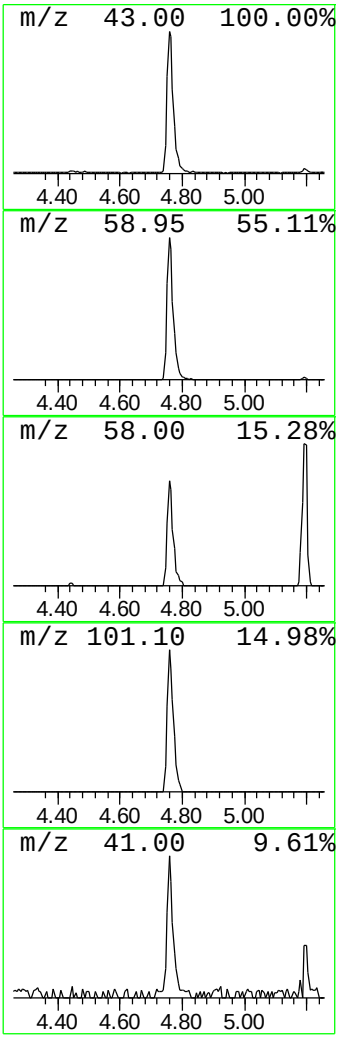
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.76	8.38 ng	243944	1,4-Dichlorobenzene-d4	6.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol	102	C6H14O	000623-37-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	28





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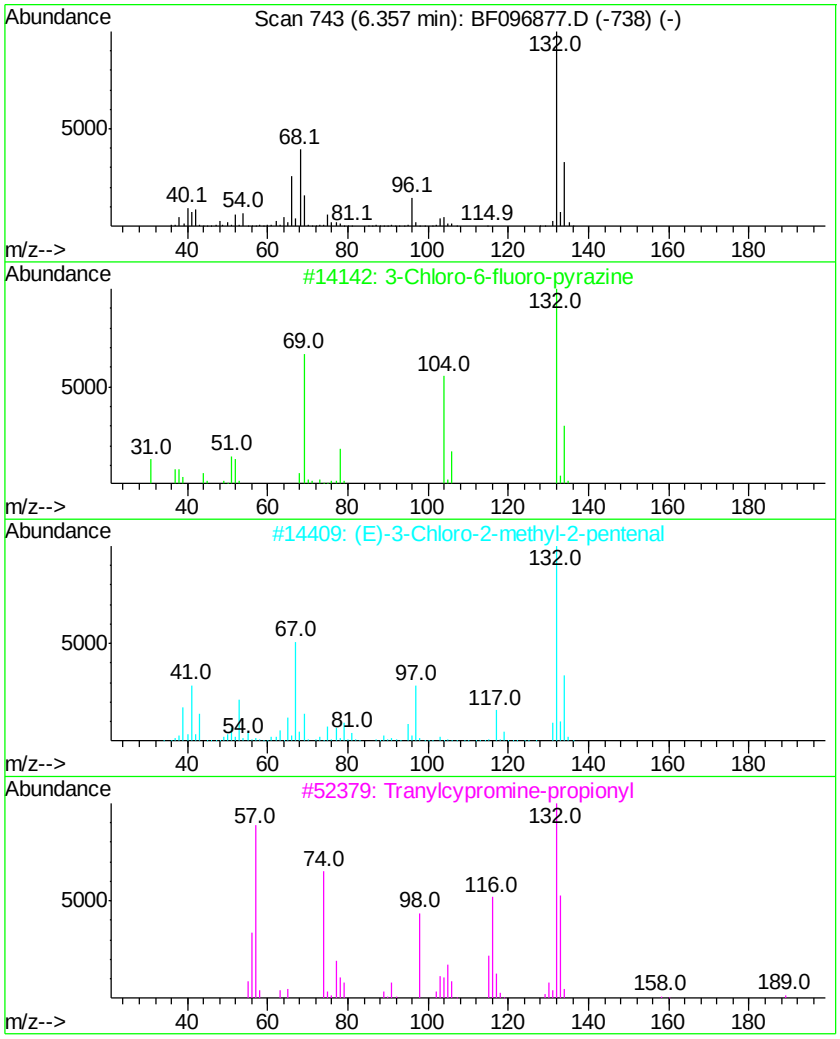
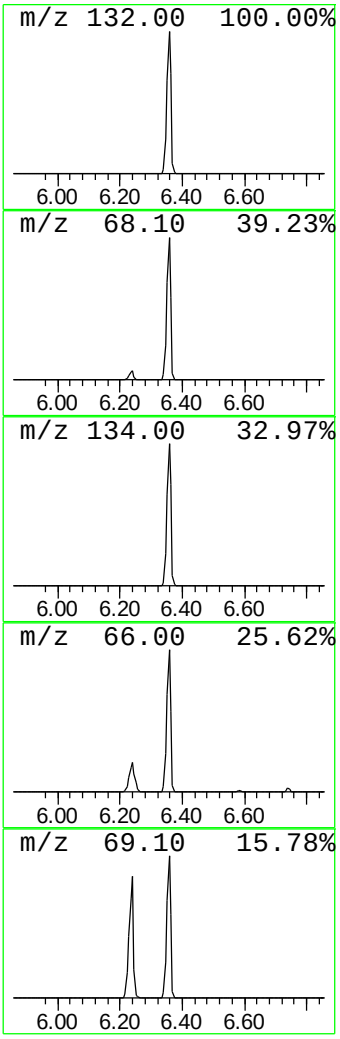
Peak Number 3 unknown6.36 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	76.28 ng	2221150	1,4-Dichlorobenzene-d4	6.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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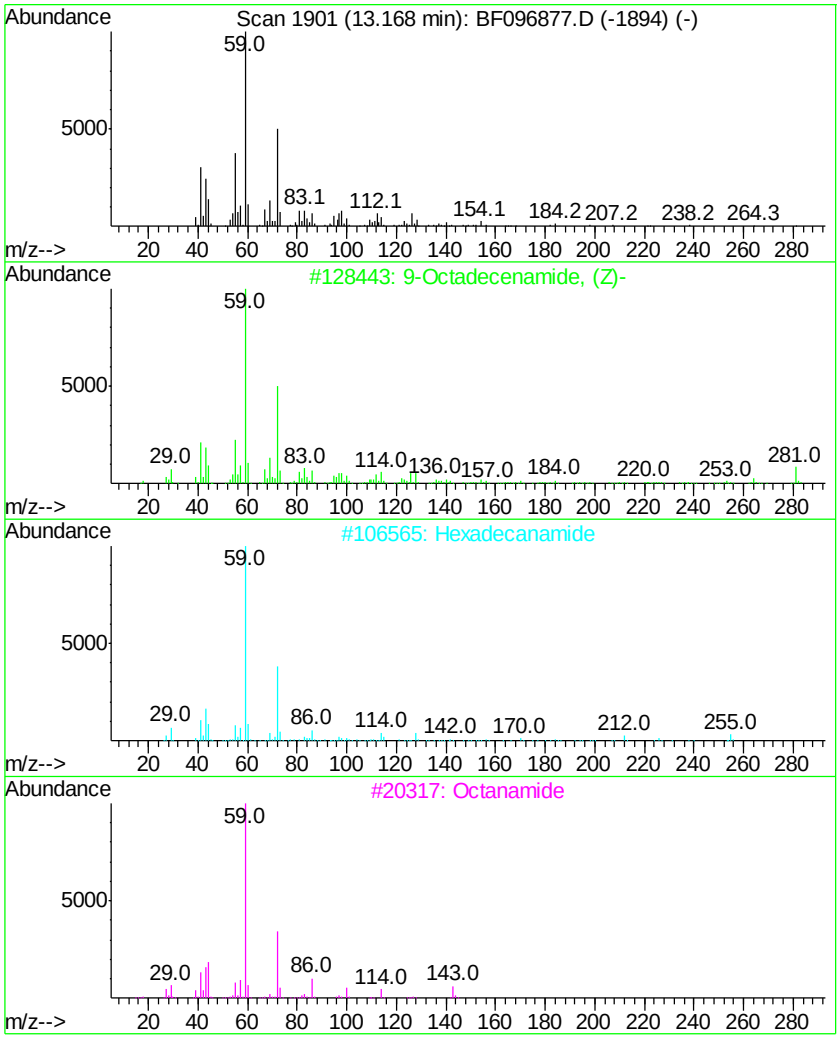
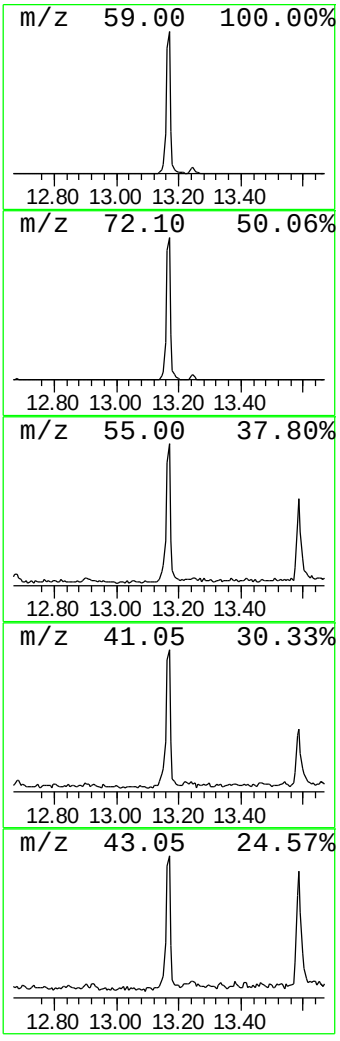
Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.17	8.30 ng	300100	Chrysene-d12	13.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2	Hexadecanamide	255	C16H33NO	000629-54-9	72
3	Octanamide	143	C8H17NO	000629-01-6	53
4	Nonanamide	157	C9H19NO	001120-07-6	53
5	Pentanamide	101	C5H11NO	000626-97-1	43





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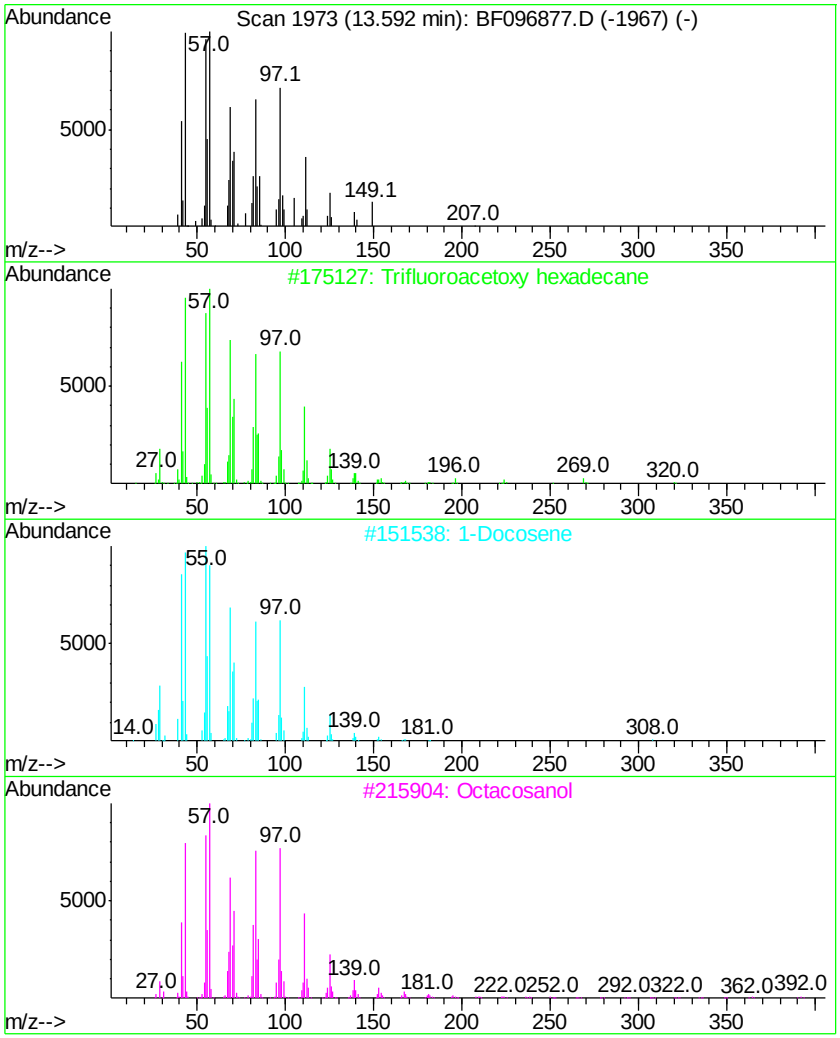
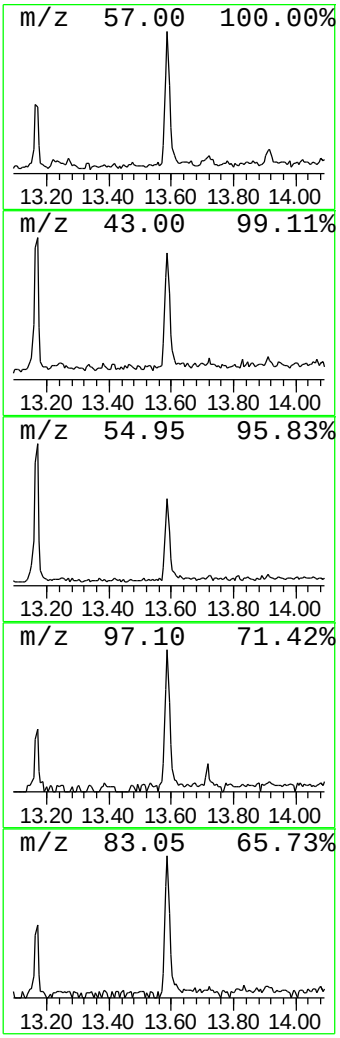
Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.59	4.27 ng	154263	Chrysene-d12	13.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2	1-Docosene	308	C22H44	001599-67-3	91
3	Octacosanol	410	C28H58O	000557-61-9	91
4	1-Heneicosanol	312	C21H44O	015594-90-8	91
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	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...	2.83	5.0	ng	146599	1	6.59	582331	20.0
2-Pentanone, 4-hy...	4.76	8.4	ng	243944	1	6.59	582331	20.0
unknown6.36	6.36	76.3	ng	2221150	1	6.59	582331	20.0
9-Octadecenamide,...	13.17	8.3	ng	300100	5	13.72	723107	20.0
Trifluoroacetoxy ...	13.59	4.3	ng	154263	5	13.72	723107	20.0