LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080817\
Data File : BF097498.D
Acq On : 9 Aug 2017 5:06
Operator : SJ/JU
Sample : I4604-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-7-080217

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-BF072517.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	4.534	464	467	483	rBV	57720	107804	4.06%	0.551%
2	5.004	544	547	572	rBV	1101420	1553647	58.46%	7.943%
3	6.081	727	730	744	rBV	678797	900022	33.86%	4.602%
4	6.181	744	747	763	rVB	2320621	2409110	90.64%	12.317%
5	6.404	782	785	798	rBV	612151	593507	22.33%	3.034%
6	6.563	808	812	830	rBV	2349150	2304998	86.73%	11.785%
7	6.981	879	883	899	rBV	1801932	1860795	70.01%	9.514%
8	7.686	1000	1003	1018	rBV	675890	709161	26.68%	3.626%
9	8.769	1183	1187	1190	rBV	2723567	2657808	100.00%	13.589%
10	9.174	1253	1256	1263	rBB	34367	30894	1.16%	0.158%
11	9.433	1296	1300	1313	rVB	813790	727171	27.36%	3.718%
12	10.221	1430	1434	1448	rBV	1311706	1267818	47.70%	6.482%
13	10.904	1547	1550	1558	rBV	589858	558732	21.02%	2.857%
14	11.139	1586	1590	1603	rBV	119942	224876	8.46%	1.150%
15	12.286	1781	1785	1792	rBV	226449	332547	12.51%	1.700%
16	12.492	1815	1820	1823	rBV	2005700	1999483	75.23%	10.223%
17	13.292	1951	1956	1967	rBV	125229	214050	8.05%	1.094%
18	13.439	1974	1981	1989	rBV	14527	31337	1.18%	0.160%
19	13.533	1993	1997	2001	rBV	562720	543716	20.46%	2.780%
20	14.174	2102	2106	2113	rBV2	49258	84251	3.17%	0.431%
21	14.874	2221	2225	2229	rBV	346573	414016	15.58%	2.117%
22	15.245	2286	2288	2294	rVB	24880	33134	1.25%	0.169%

Sum of corrected areas: 19558877

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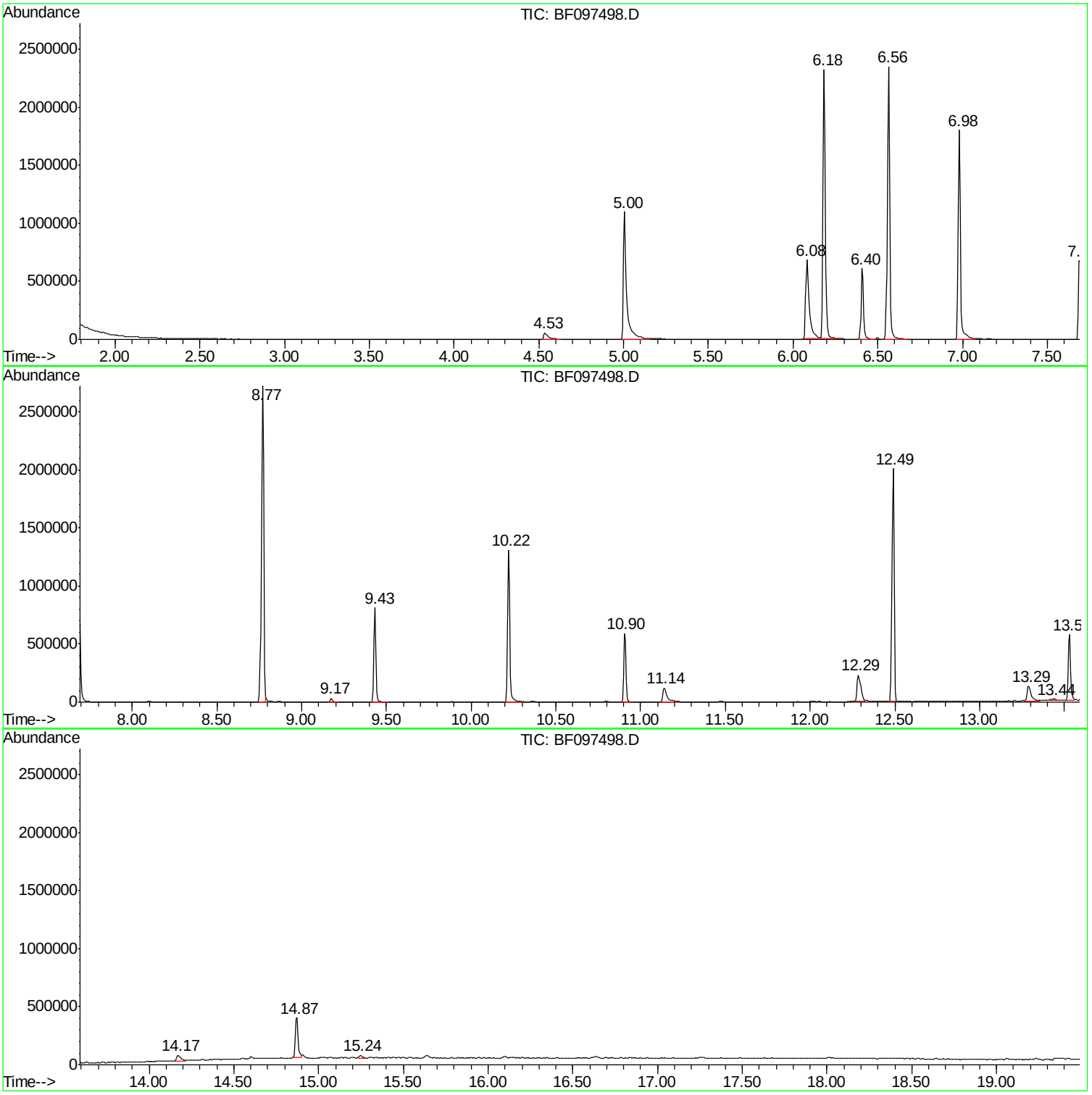
MW-7-080217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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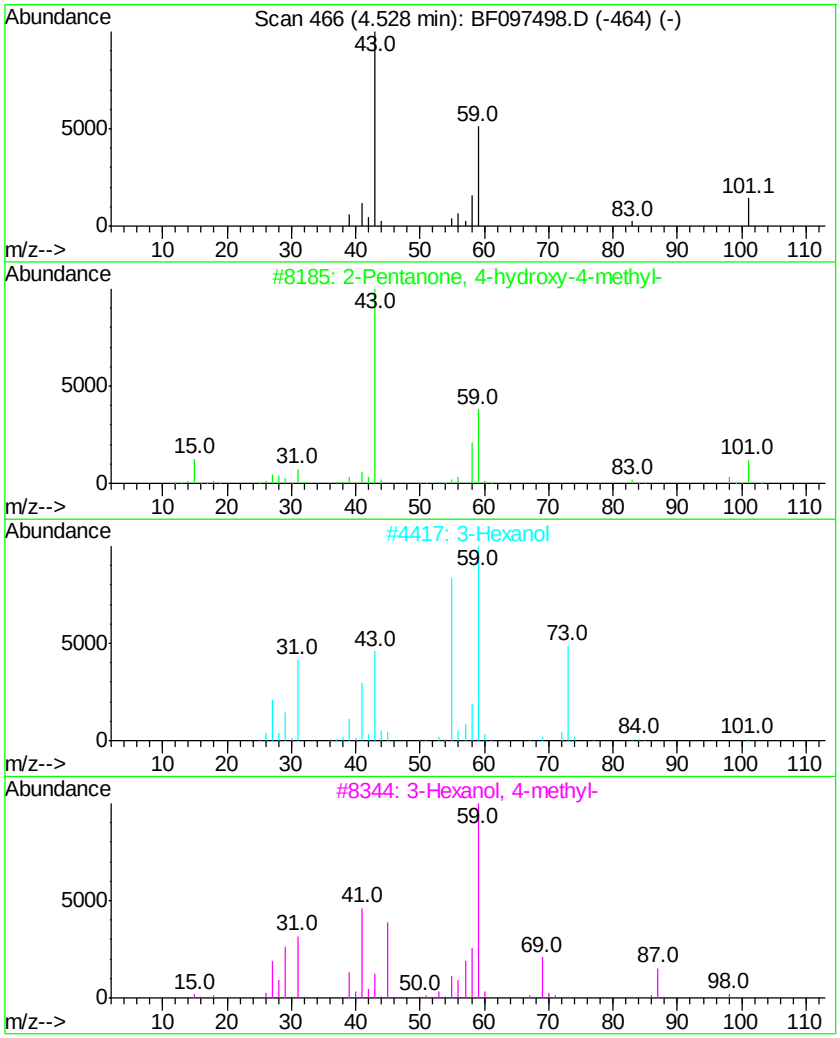
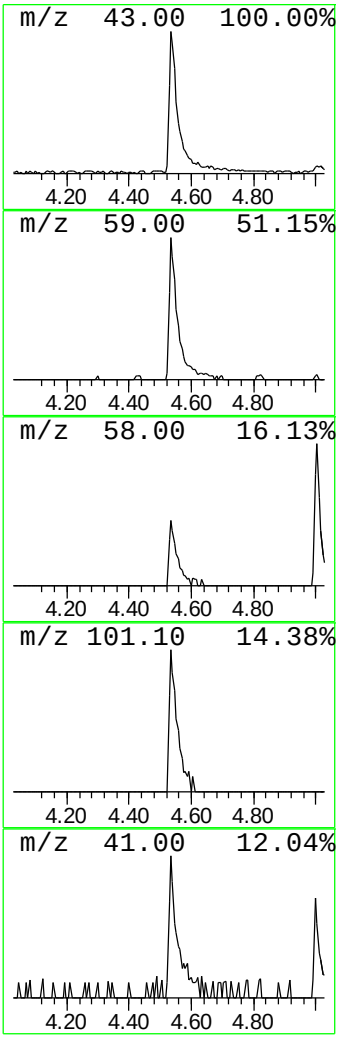
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.53	3.63 ng	107804	1,4-Dichlorobenzene-d4	6.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	3-Hexanol	102	C6H14O	000623-37-0	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
5	1,3,4-Oxadiazole, 2-(acetyloxy)-...	172	C7H12N2O3	066398-57-0	12





Library Search Compound Report

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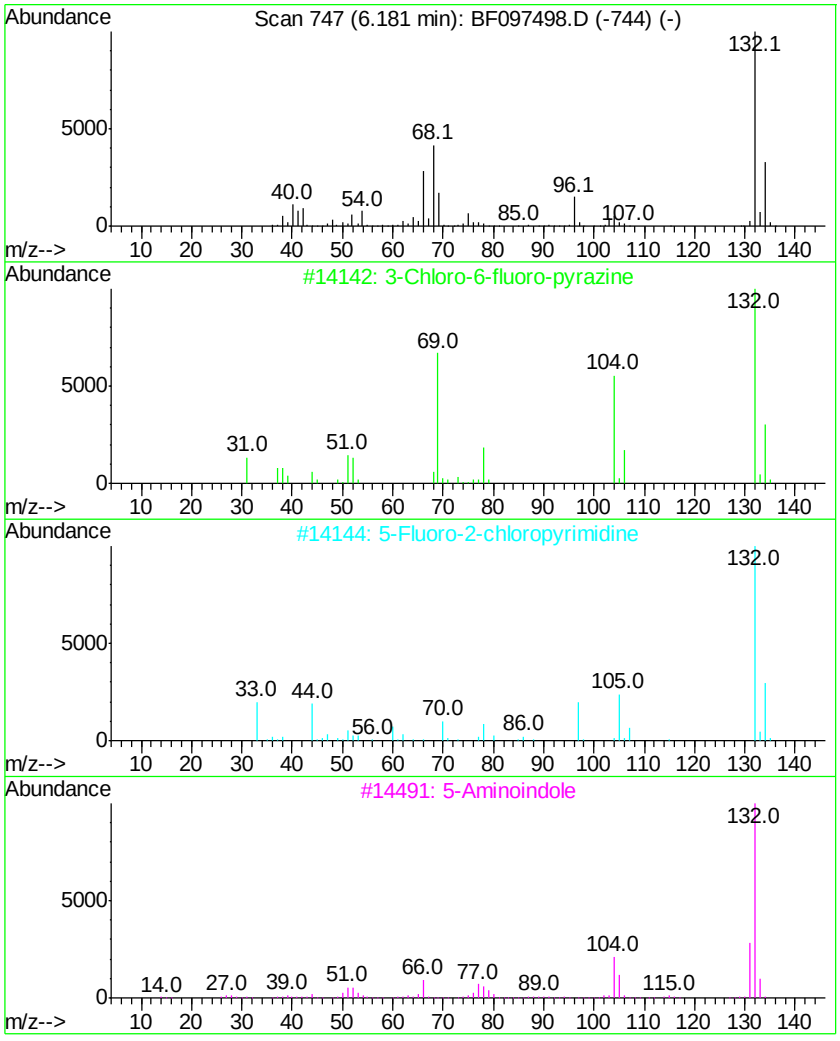
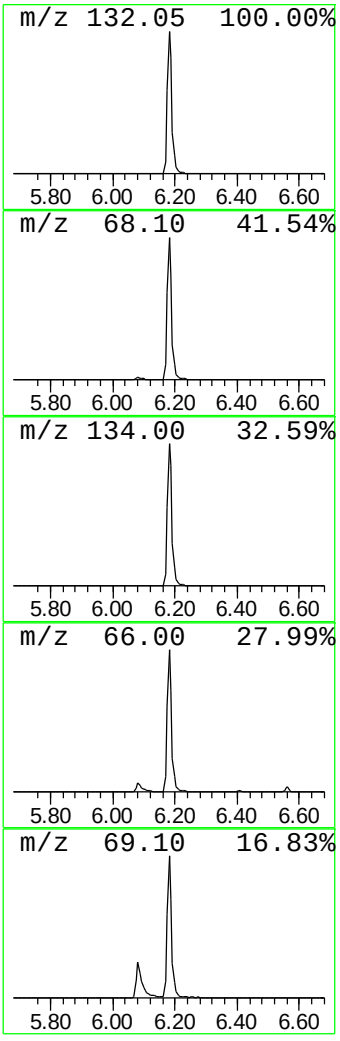
****

Peak Number 2 unknown6.18 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.18	81.18 ng	2409110	1,4-Dichlorobenzene-d4	6.40

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-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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ClientSampleId : MW-7-080217

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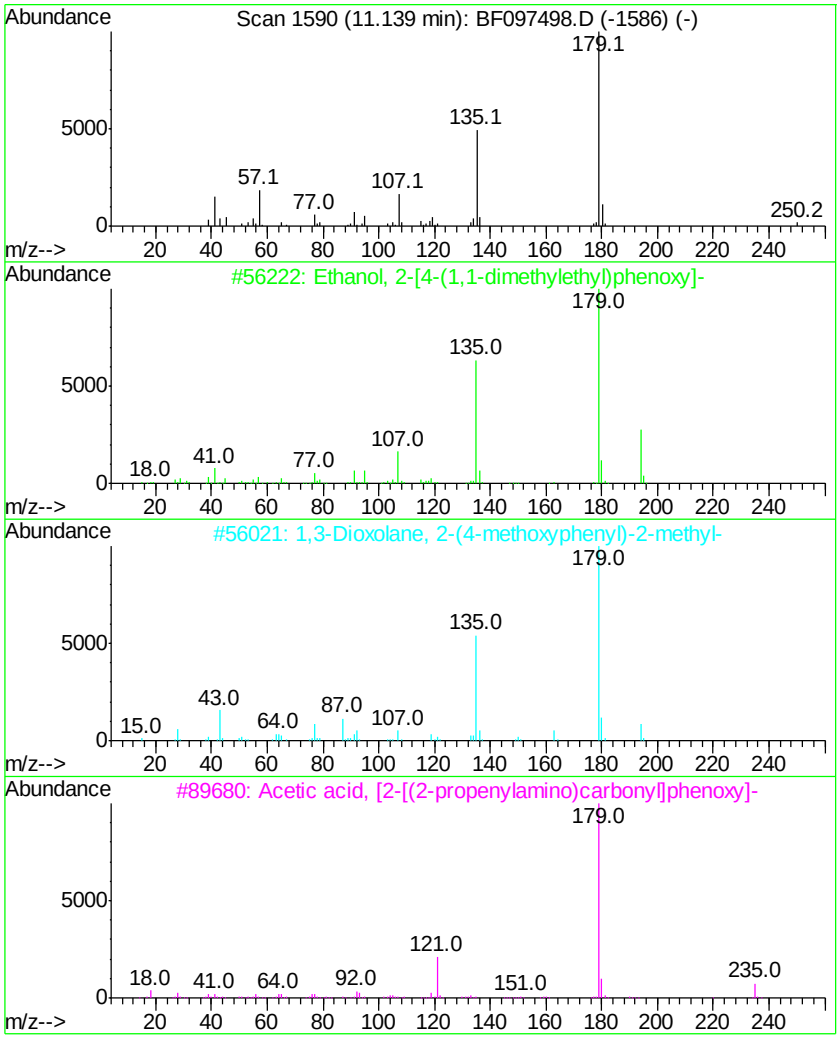
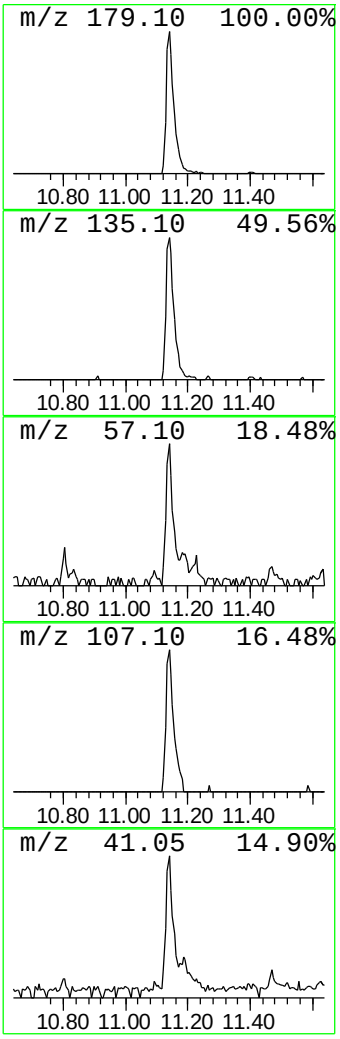
****
Peak Number 4 Ethanol, 2-[4-(1,1-dimethyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.14	8.05 ng	224876	Phenanthrene-d10	10.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[4-(1,1-dimethylethyl...	194	C12H18O2	000713-46-2	86
2	1,3-Dioxolane, 2-(4-methoxypheny...	194	C11H14O3	036881-00-2	56
3	Acetic acid, [2-[(2-propenylamin...	235	C12H13NO4	000119-45-9	37
4	4-tert-Butyl-2-nitroacetanilide	236	C12H16N2O3	040655-37-6	23
5	(p-(Allyloxycarbonyl)phenoxy)ace...	236	C12H12O5	1000241-83-7	23





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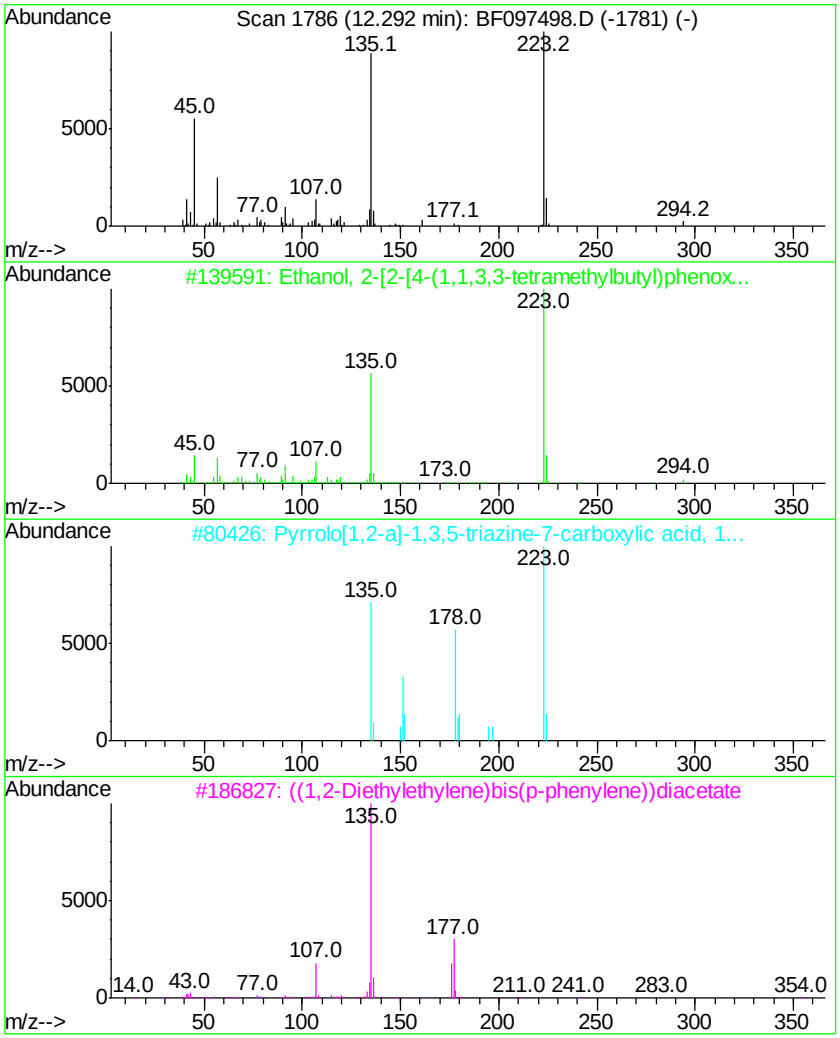
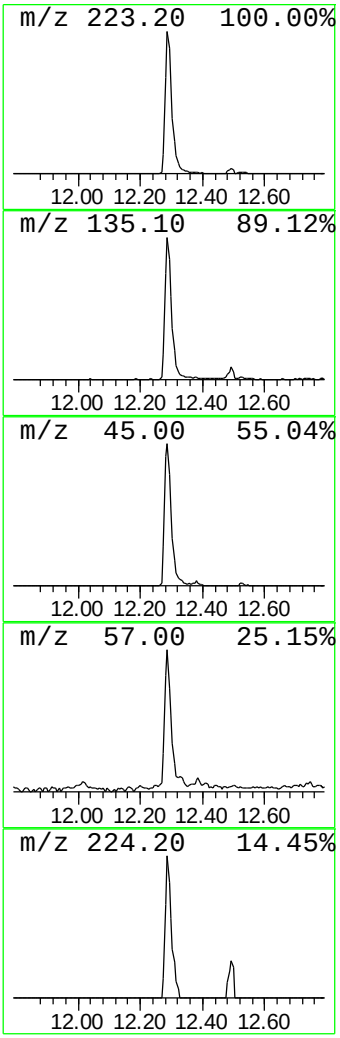
****

Peak Number 5 Ethanol, 2-[2-[4-(1,1,3,3-t... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	12.23 ng	332547	Chrysene-d12	13.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	92
2	Pyrrolo[1,2-a]-1,3,5-triazine-7-...	223	C9H9N3O4	054449-89-7	90
3	((1,2-Diethylethylene)bis(p-phen...	354	C22H26O4	004547-76-6	35
4	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	27
5	1,4-Benzenediamine, N-(1-methylh...	220	C14H24N2	039563-50-3	27





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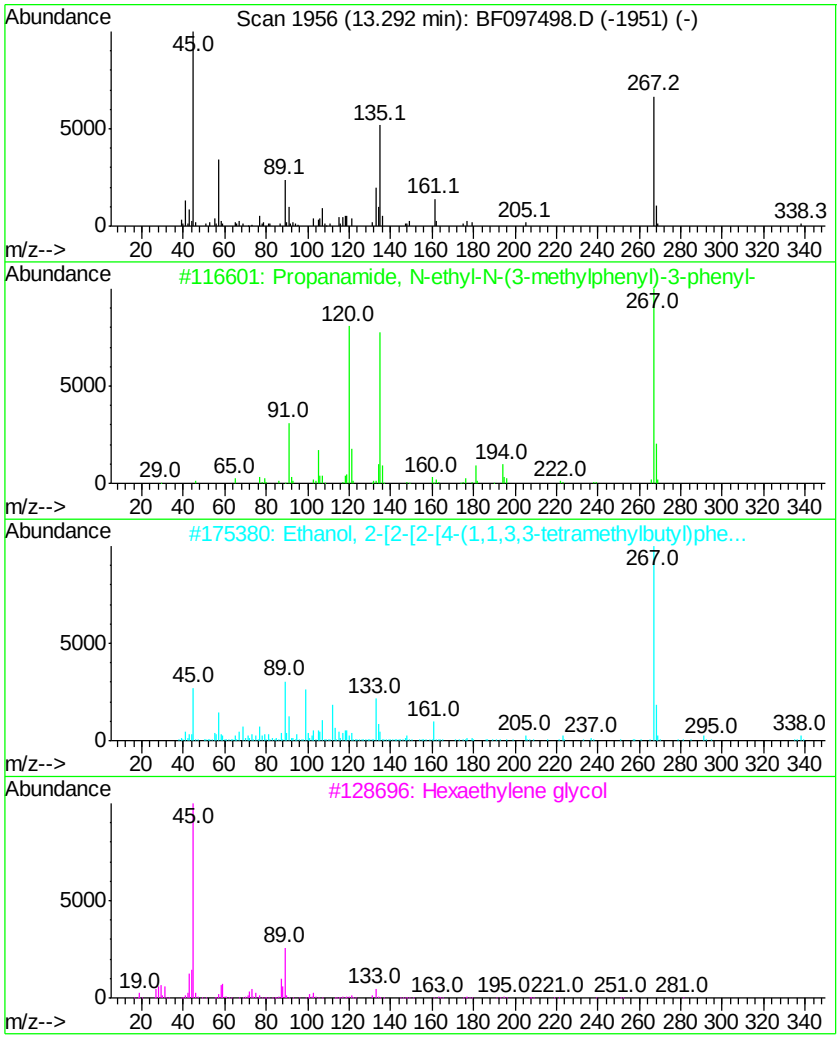
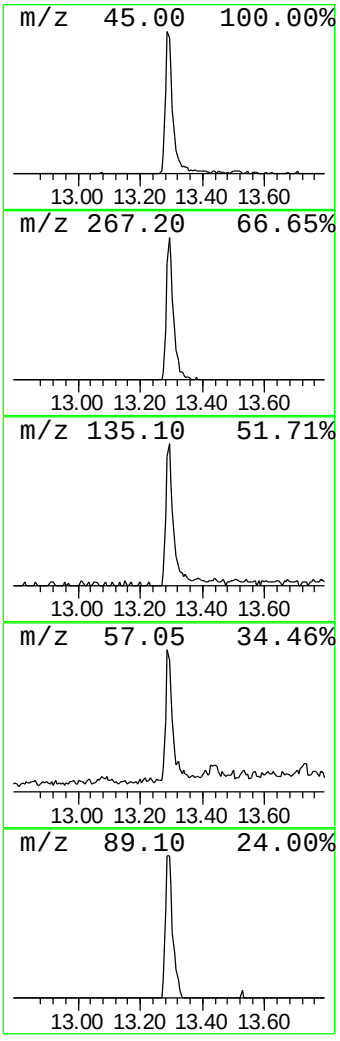
****

Peak Number 6 unknown13.29 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.29	7.87 ng	214050	Chrysene-d12	13.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanamide, N-ethyl-N-(3-methyl...	267	C18H21NO	1000308-21-3	49
2	Ethanol, 2-[2-[2-[4-(1,1,3,3-tet...	338	C20H34O4	002315-62-0	46
3	Hexaethylene glycol	282	C12H26O7	002615-15-8	38
4	Heptaethylene glycol	326	C14H30O8	005617-32-3	32
5	Phenelzine	136	C8H12N2	000051-71-8	12





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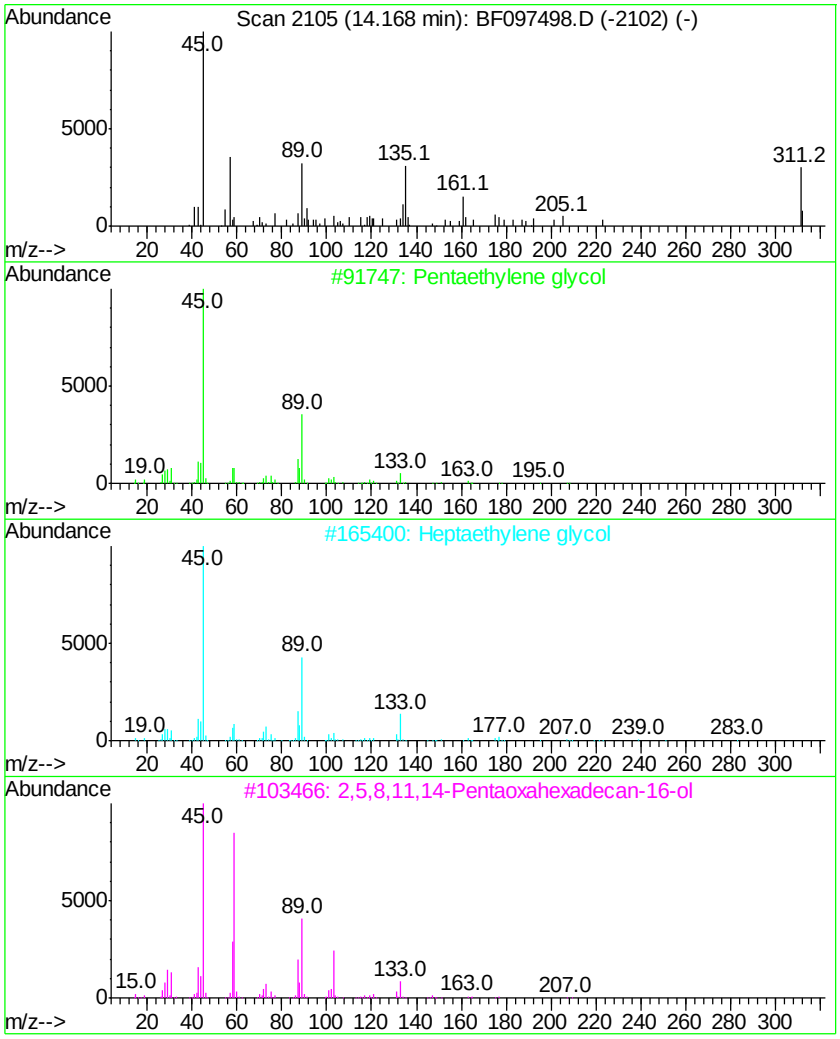
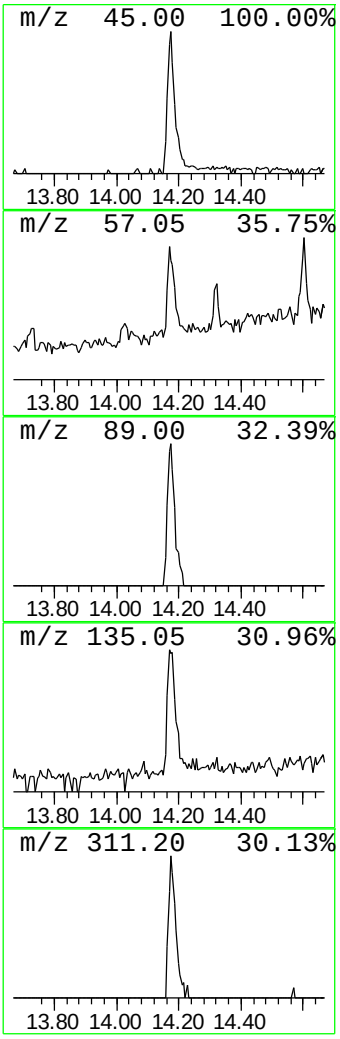
****

Peak Number 7 unknown14.17 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.17	3.10 ng	84251	Chrysene-d12	13.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentaethylene glycol	238	C10H22O6	004792-15-8	25
2	Heptaethylene glycol	326	C14H30O8	005617-32-3	25
3	2,5,8,11,14-Pentaoxahexadecan-16-ol	252	C11H24O6	023778-52-1	25
4	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	23
5	Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	23





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.53	3.6	ng	107804	1	6.40	593507	20.0
unknown6.18	6.18	81.2	ng	2409110	1	6.40	593507	20.0
Ethanol, 2-[4-(1,...	11.14	8.1	ng	224876	4	10.90	558732	20.0
Ethanol, 2-[2-[4-...	12.29	12.2	ng	332547	5	13.53	543716	20.0
unknown13.29	13.29	7.9	ng	214050	5	13.53	543716	20.0
unknown14.17	14.17	3.1	ng	84251	5	13.53	543716	20.0