LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110116\
Data File : BF090955.D
Acq On : 1 Nov 2016 17:15
Operator : UM/SJ
Sample : H5478-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SD-1

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-BF102616.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	4.899	243	246	255	rBV	679918	961882	19.15%	2.294%
2	5.333	281	284	287	rBV	3612683	3752441	74.70%	8.947%
3	6.384	373	376	378	rBV	3415248	4302846	85.66%	10.260%
4	6.499	384	386	389	rBV	3129479	4181794	83.25%	9.971%
5	6.739	405	407	409	rBV	797810	933679	18.59%	2.226%
6	6.887	418	420	423	rBV	2822095	3058330	60.88%	7.292%
7	7.299	454	456	459	rBV	2061860	2420957	48.19%	5.773%
8	7.413	463	466	471	rVB	82890	148643	2.96%	0.354%
9	8.019	517	519	522	rBV	1353933	1348935	26.85%	3.216%
10	9.105	611	614	616	rBV	4664070	5023257	100.00%	11.977%
11	9.493	646	648	651	rBV	911025	1249078	24.87%	2.978%
12	9.699	662	666	670	rBV2	26934	73433	1.46%	0.175%
13	9.779	670	673	675	rBV	1132228	1579310	31.44%	3.766%
14	10.213	703	711	713	rBV3	62262	129055	2.57%	0.308%
15	10.431	727	730	734	rBV	25898	53766	1.07%	0.128%
16	10.568	739	742	744	rBV	2613915	3226946	64.24%	7.694%
17	10.682	751	752	757	rVB	82571	141350	2.81%	0.337%
18	11.139	789	792	793	rBV	69111	75672	1.51%	0.180%
19	11.253	800	802	805	rBV	1787106	1626760	32.38%	3.879%
20	11.311	805	807	812	rVB2	25725	58009	1.15%	0.138%
21	12.842	938	941	944	rBV	4388133	4574502	91.07%	10.907%
22	13.745	1017	1020	1030	rBV2	168901	242391	4.83%	0.578%
23	13.894	1030	1033	1035	rBV	949942	1356619	27.01%	3.235%
24	14.374	1073	1075	1080	rBV	43914	54181	1.08%	0.129%
25	14.740	1105	1107	1109	rVB	49571	64304	1.28%	0.153%
26	14.980	1126	1128	1133	rVB	80388	93527	1.86%	0.223%
27	15.288	1152	1155	1157	rBV	735763	933564	18.58%	2.226%
28	15.722	1190	1193	1195	rBV	130106	204484	4.07%	0.488%
29	16.705	1275	1279	1283	rBV	32802	69762	1.39%	0.166%

Sum of corrected areas: 41939477

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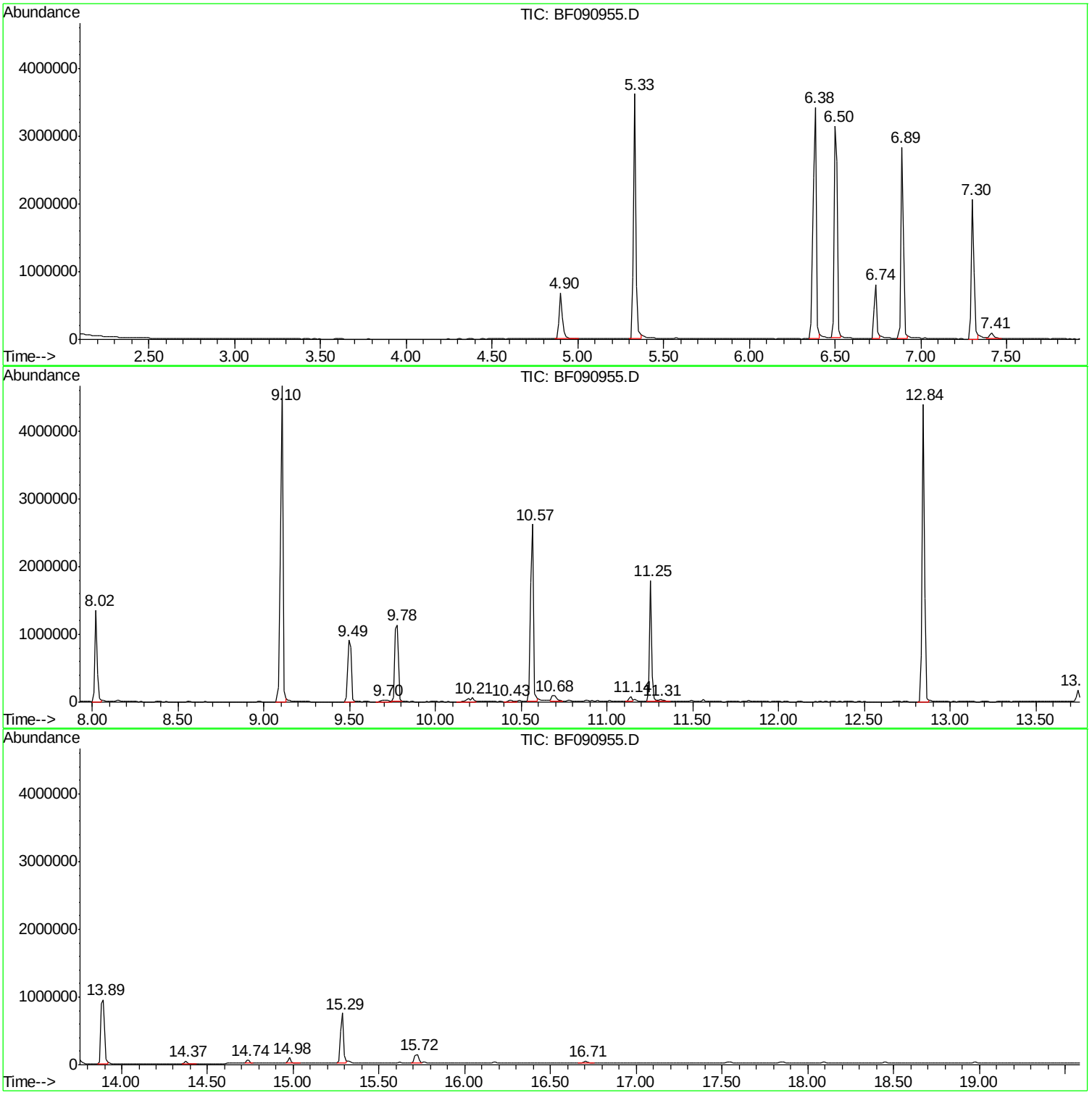
Instrument : BNA_F
ClientSampleId : SD-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : SD-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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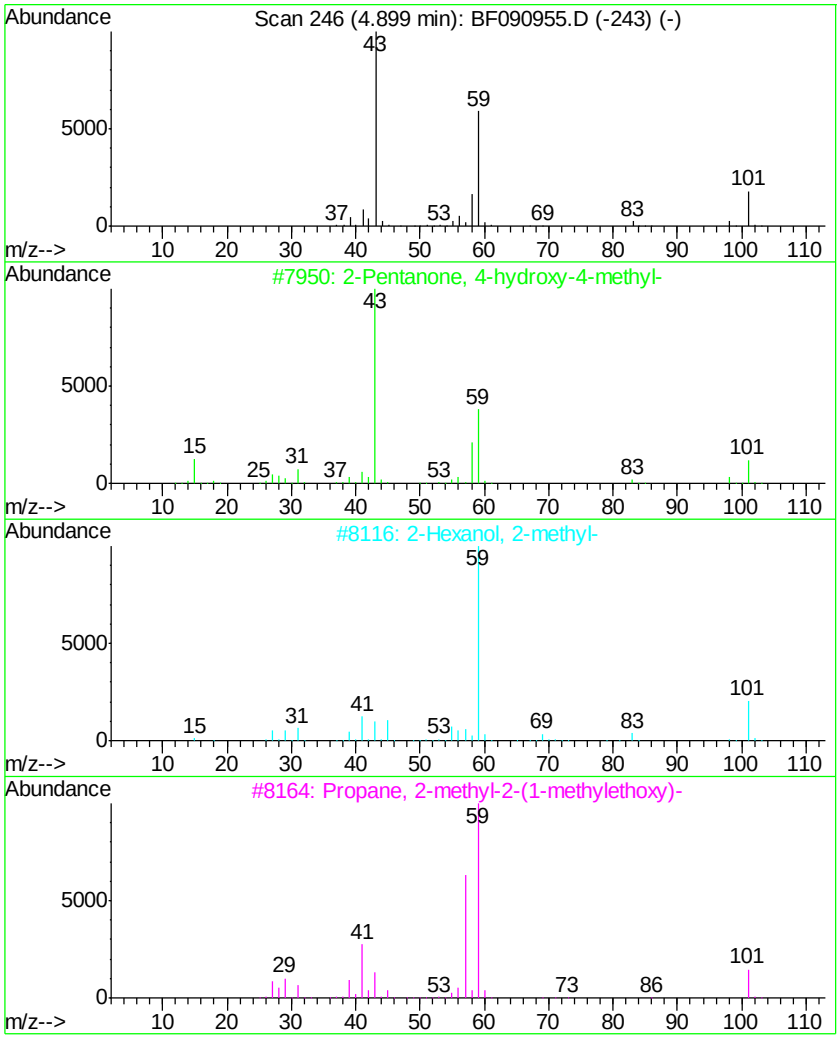
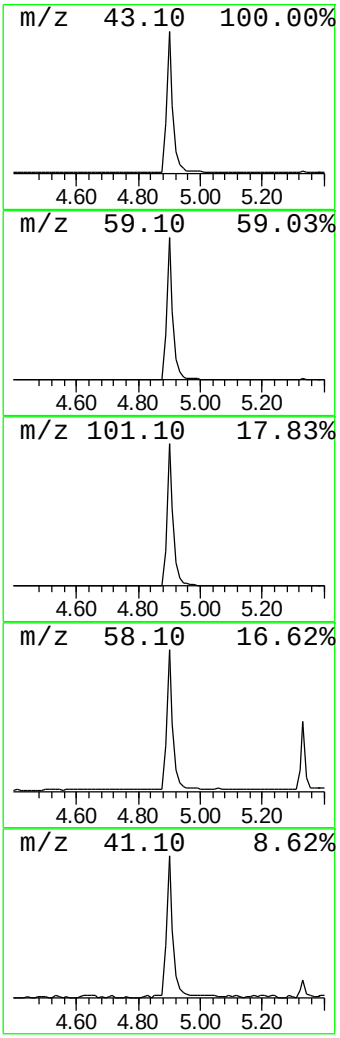
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	20.60 ng	961882	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Sample : H5478-01
Misc :
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Instrument : BNA_F
ClientSampleId : SD-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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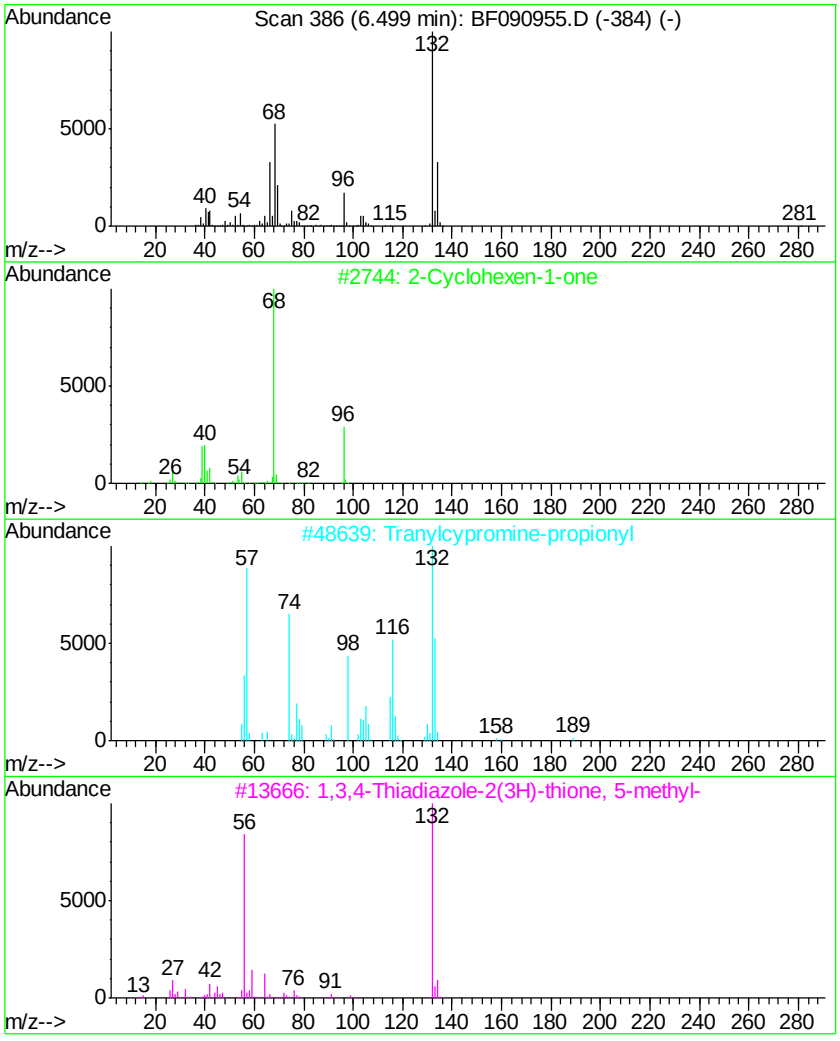
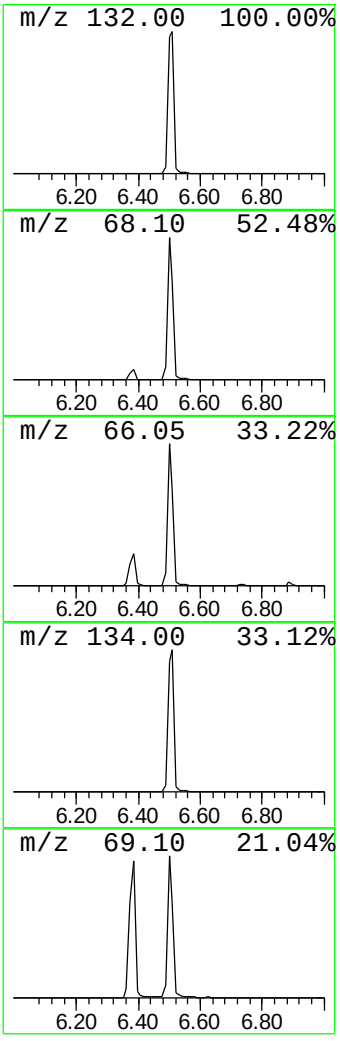
Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	89.58 ng	4181790	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
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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Instrument : BNA_F
ClientSampleId : SD-1

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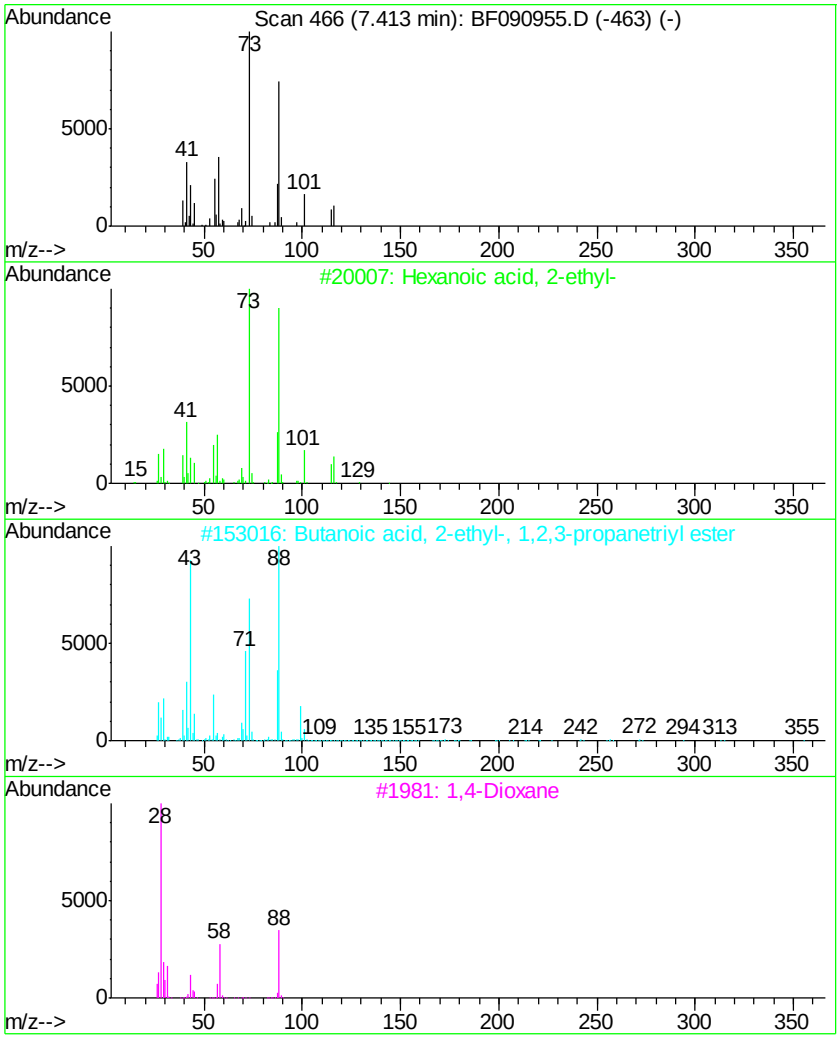
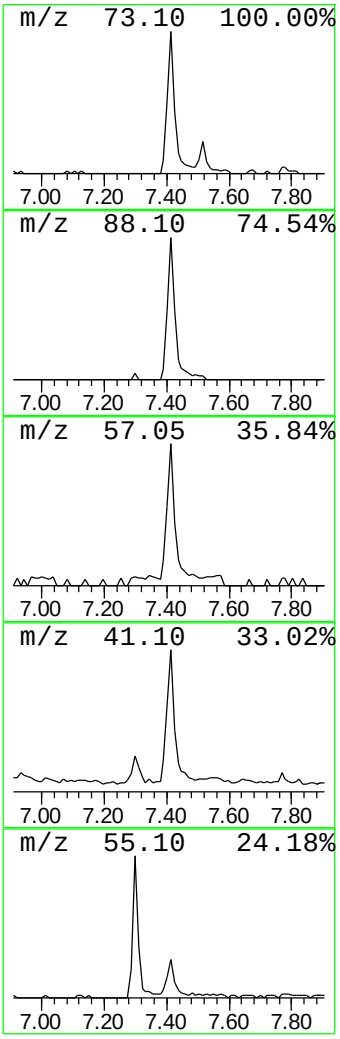
Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	2.20 ng	148643	Naphthalene-d8	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	45
3	1,4-Dioxane	88	C4H8O2	000123-91-1	43
4	Hexanamide, 6-(heptyloxy)-	229	C13H27NO2	055191-08-7	40
5	Methyl L-(+)-.beta.-hydroxyisobu...	118	C5H10O3	080657-57-4	33





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ClientSampleId : SD-1

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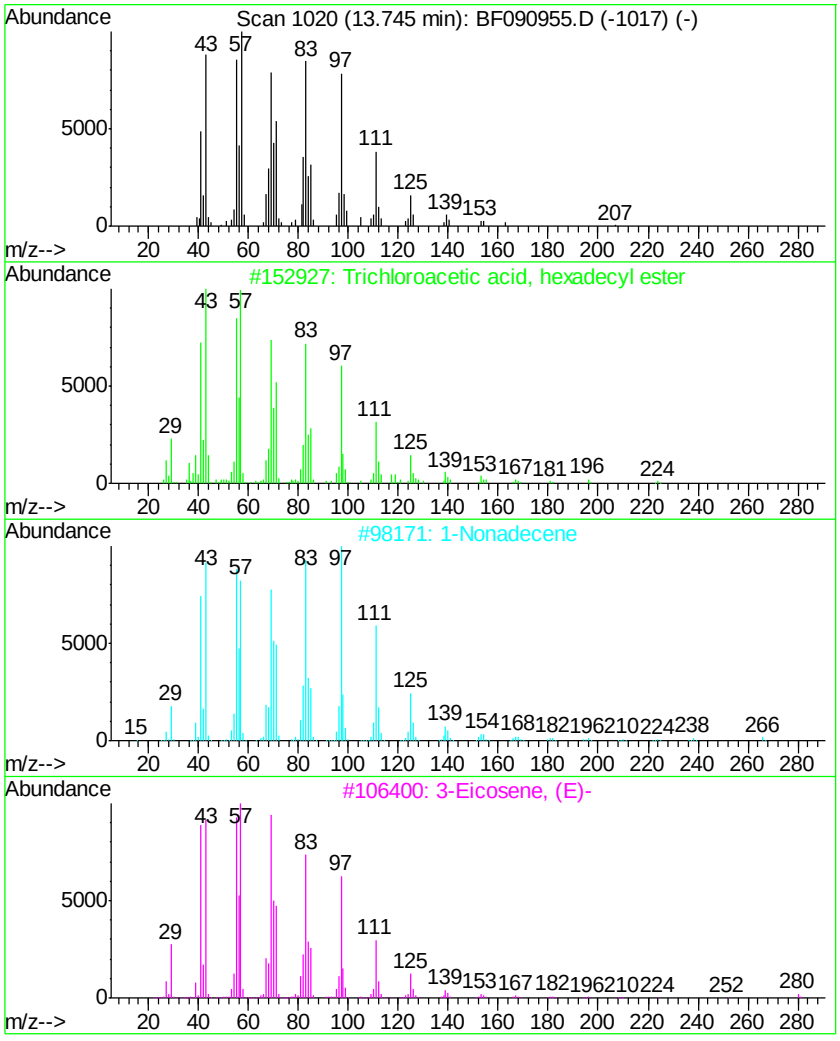
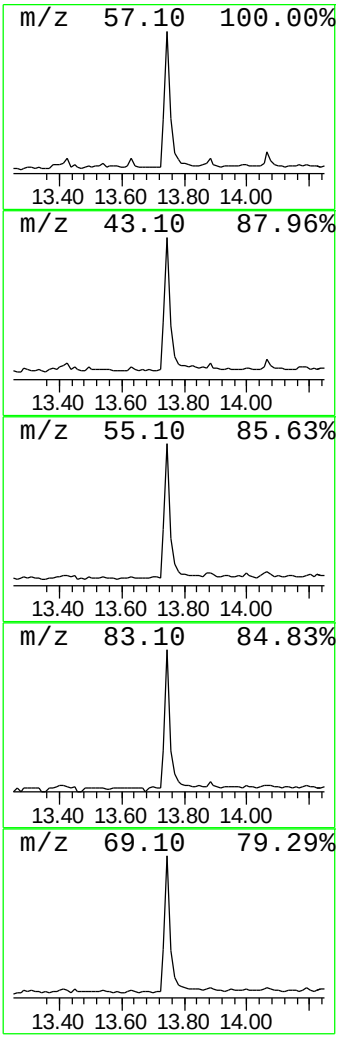
Peak Number 5 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	3.57 ng	242391	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90





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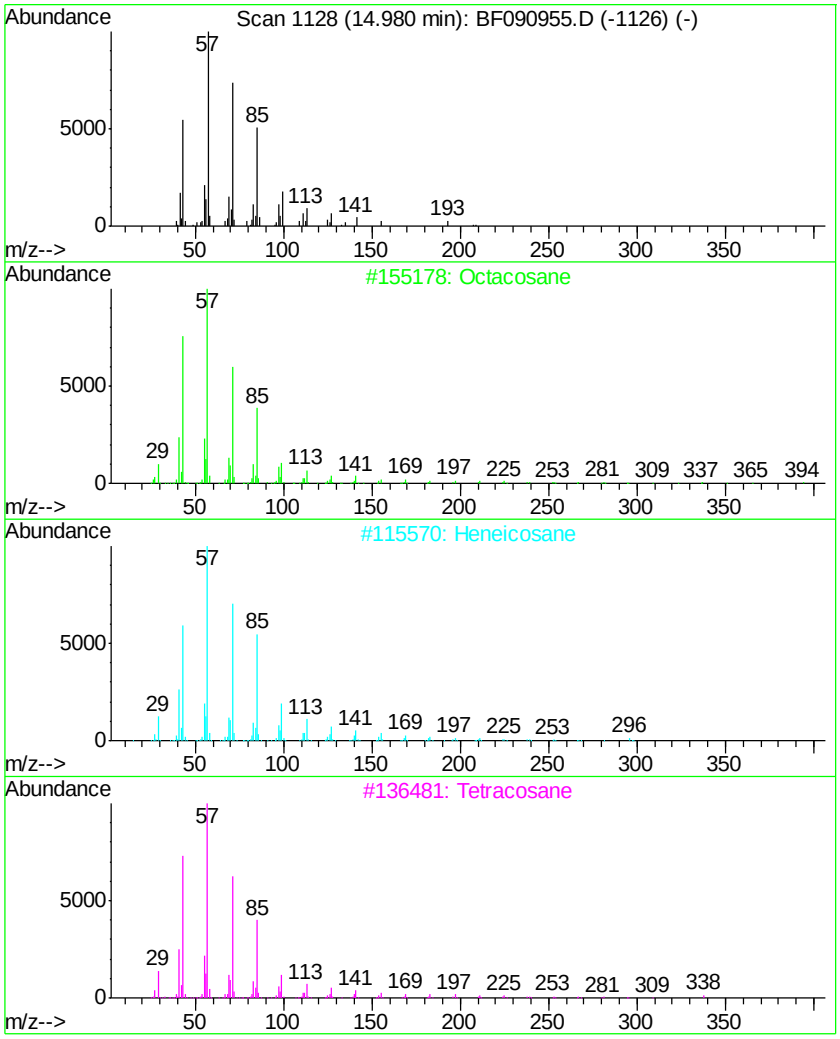
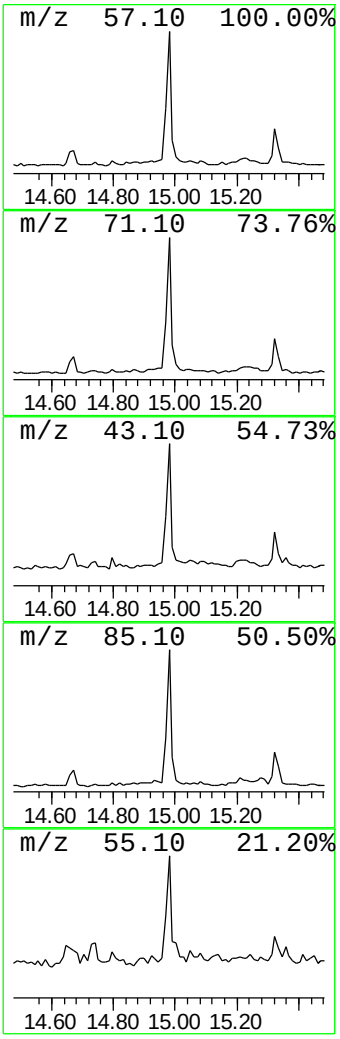
Peak Number 6 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	2.00 ng	93527	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetracosane	338	C24H50	000646-31-1	90
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	86
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86





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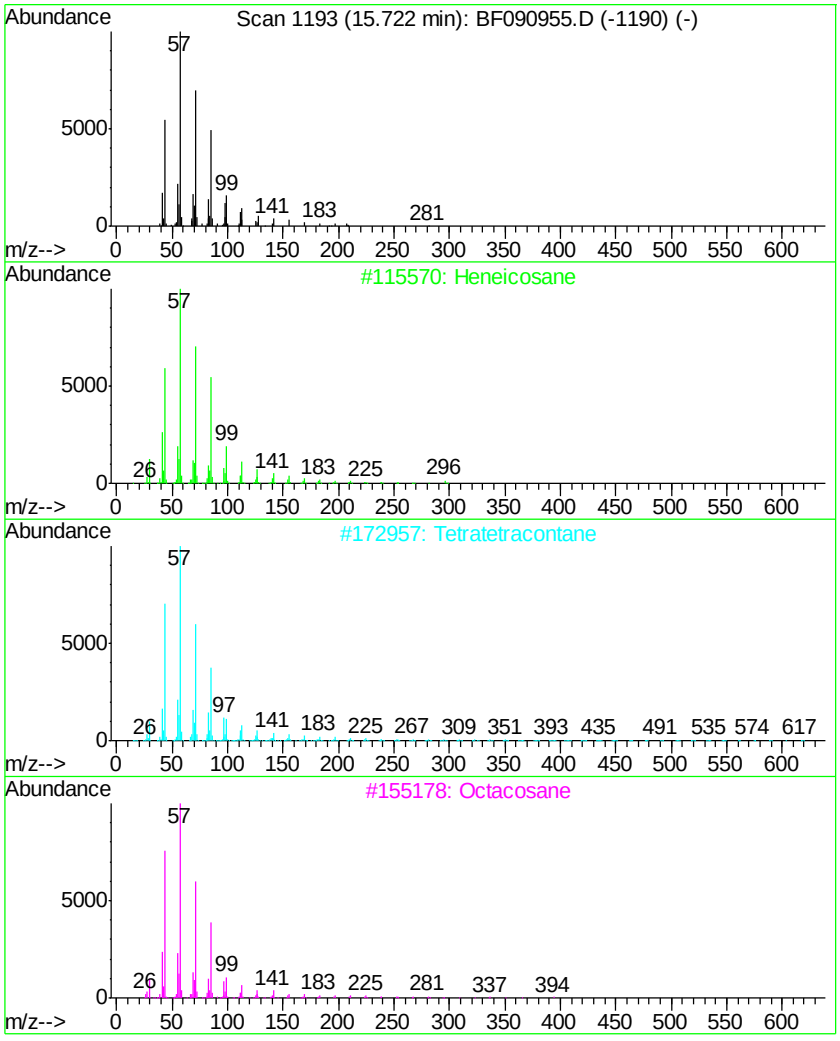
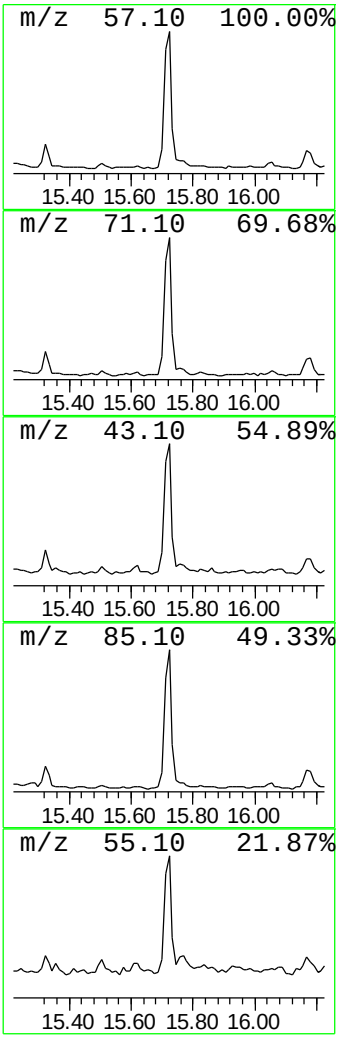
Peak Number 7 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	4.38 ng	204484	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tetratetracontane	619	C44H90	007098-22-8	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Triacontane	422	C30H62	000638-68-6	90
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	86





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	20.6	ng	961882	1	6.74	933679	20.0
unknown6.50	6.50	89.6	ng	4181790	1	6.74	933679	20.0
Hexanoic acid, 2-...	7.41	2.2	ng	148643	2	8.02	1348940	20.0
Trichloroacetic a...	13.75	3.6	ng	242391	5	13.89	1356620	20.0
Octacosane	14.98	2.0	ng	93527	6	15.29	933564	20.0
Heneicosane	15.72	4.4	ng	204484	6	15.29	933564	20.0