LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070716\
Data File : BF088810.D
Acq On : 8 Jul 2016 6:54
Operator : UM/SJ
Sample : H3897-10
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-12-COMP

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	1.690	8	9	19	rVB	260003	488074	12.43%	2.526%
2	1.815	19	20	69	rVB	1727753	3925777	100.00%	20.319%
3	4.902	287	290	294	rBV	68539	103133	2.63%	0.534%
4	5.187	313	315	317	rBV2	124688	178628	4.55%	0.925%
5	5.244	317	320	321	rVV2	42376	108953	2.78%	0.564%
6	5.336	325	328	330	rBV	1511820	1519234	38.70%	7.863%
7	5.450	335	338	342	rVB	26119	48444	1.23%	0.251%
8	6.376	416	419	422	rBV	1090331	1508479	38.42%	7.807%
9	6.513	428	431	433	rBV	1328626	1593428	40.59%	8.247%
10	6.627	439	441	443	rBB	321119	369137	9.40%	1.911%
11	6.742	449	451	453	rBB	593467	483439	12.31%	2.502%
12	6.902	462	465	467	rBB	1125556	1214024	30.92%	6.283%
13	7.302	497	500	503	rBV	878483	858787	21.88%	4.445%
14	8.022	561	563	566	rBV	562730	564247	14.37%	2.920%
15	8.536	607	608	611	rBB	95049	94719	2.41%	0.490%
16	9.108	655	658	660	rBV	2042982	1799905	45.85%	9.316%
17	9.496	690	692	695	rBV	179335	162557	4.14%	0.841%
18	9.782	714	717	719	rBV	460379	553923	14.11%	2.867%
19	10.559	783	785	788	rBV	765673	764031	19.46%	3.954%
20	11.256	843	846	848	rVB	572440	499116	12.71%	2.583%
21	12.674	968	970	973	rBB2	37524	49011	1.25%	0.254%
22	12.845	982	985	987	rBV	1227137	1424788	36.29%	7.374%
23	13.748	1062	1064	1070	rBV	55813	103673	2.64%	0.537%
24	13.885	1073	1076	1078	rBV	465745	531538	13.54%	2.751%
25	15.268	1194	1197	1200	rBV	329390	374101	9.53%	1.936%

Sum of corrected areas: 19321146

LSC Report - Integrated Chromatogram

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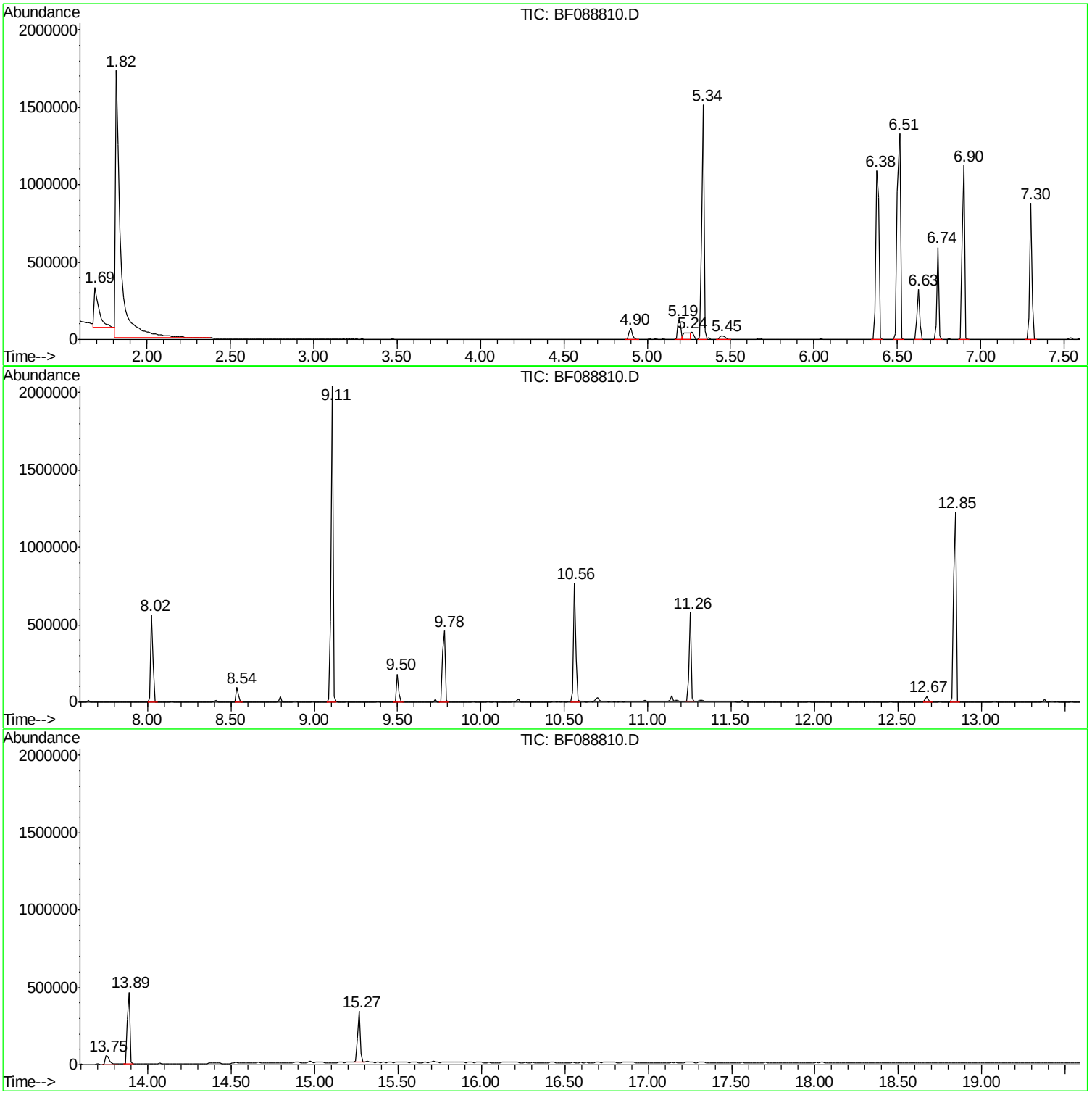
Instrument : BNA_F
ClientSampleId : SB-12-COMP

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

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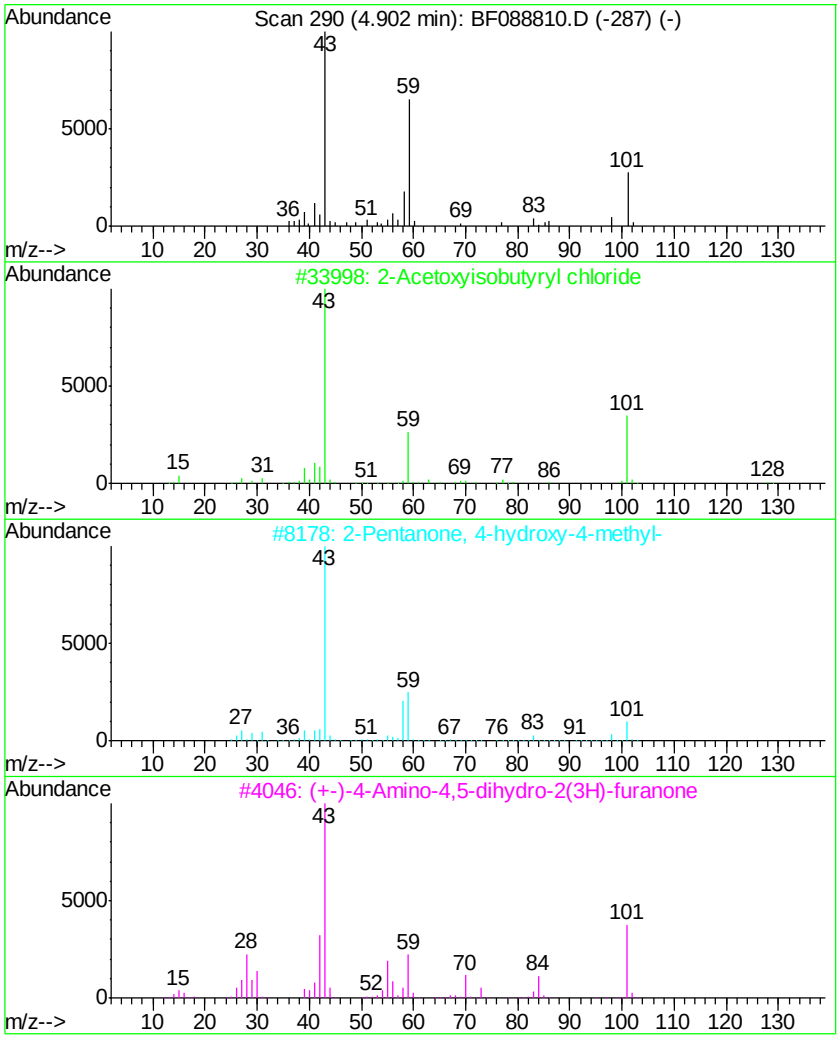
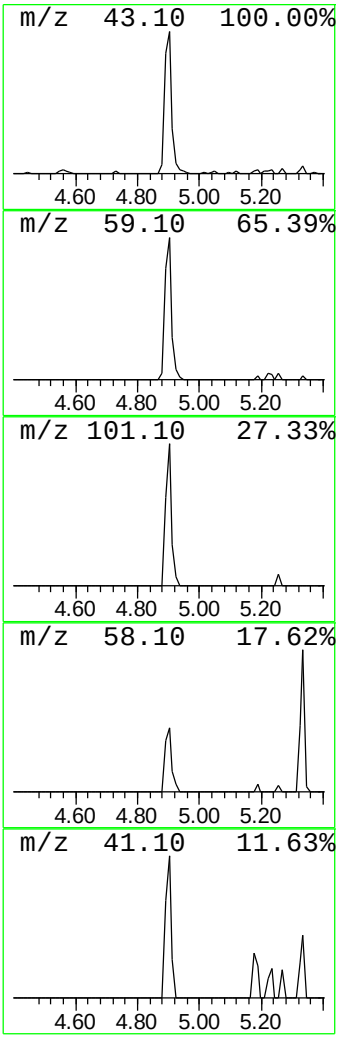
Peak Number 3 2-Acetoxyisobutyryl chloride Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	4.27 ng	103133	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Acetoxyisobutyryl chloride	164	C6H9ClO3	040635-66-3	64
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	53
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	27





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ClientSampleId : SB-12-COMP

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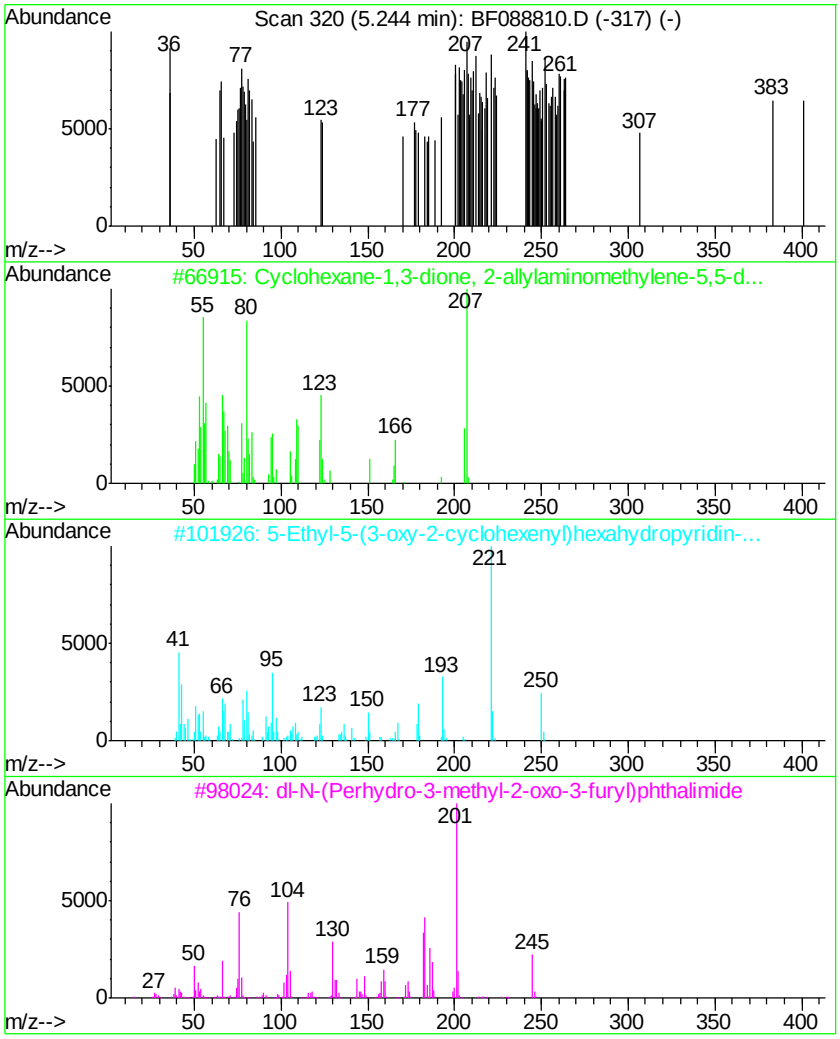
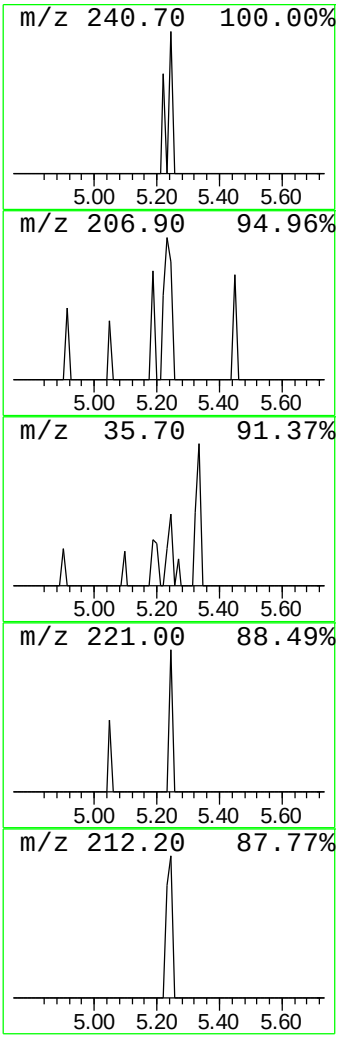
Peak Number 5 unknown5.24 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	4.51 ng	108953	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane-1,3-dione, 2-allylam...	207	C12H17NO2	104926-37-6	30
2	5-Ethyl-5-(3-oxy-2-cyclohexenyl)...	250	C12H14N2O4	1000322-46-7	30
3	dl-N-(Perhydro-3-methyl-2-oxo-3-...	245	C13H11NO4	1000243-90-3	27
4	Thiophene, 2-(3-nitrophenylimino...	246	C12H10N2O2S	314279-45-3	27
5	Tricyclo[4.2.1.0(2,5)]nonan-3-on...	204	C9H10Cl2O	068295-68-1	16





Library Search Compound Report

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Sample : H3897-10
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
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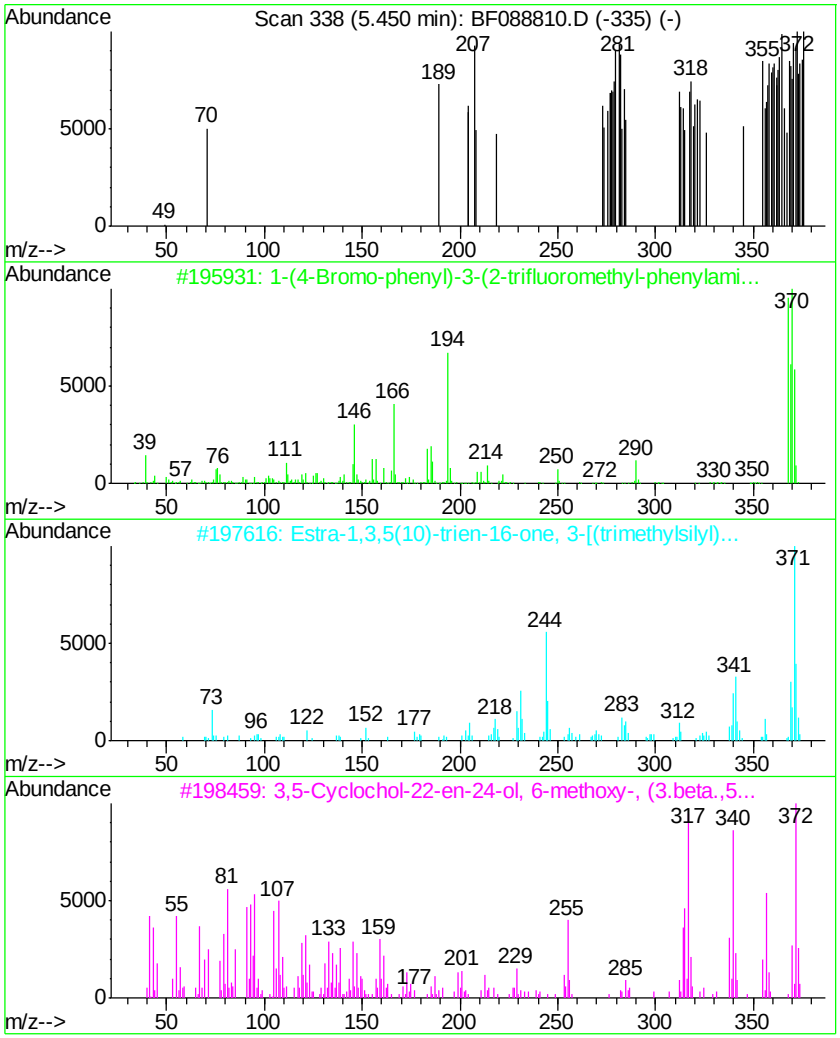
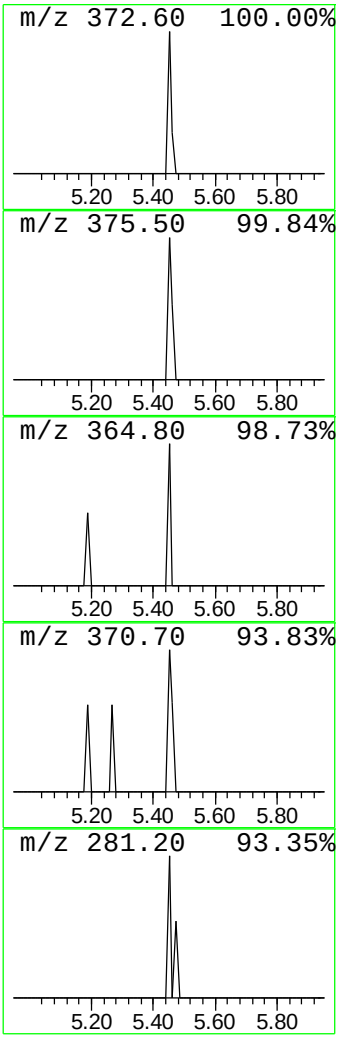
Peak Number 6 unknown5.45 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.45	2.00 ng	48444	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(4-Bromo-phenyl)-3-(2-trifluor...	369	C16H11BrF3NO	1000295-87-3	27
2	Estra-1,3,5(10)-trien-16-one, 3-...	371	C22H33NO2Si	077904-50-8	16
3	3,5-Cyclochol-22-en-24-ol, 6-met...	372	C25H40O2	056259-13-3	15
4	5,5'-Dibromo-2,2'-dimethoxy-diph...	370	C14H12Br2O2	1000318-03-1	14
5	9-Chloro-7-(4-methylpiperazino)-...	363	C22H22ClN3	1000326-78-5	10





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Instrument : BNA_F
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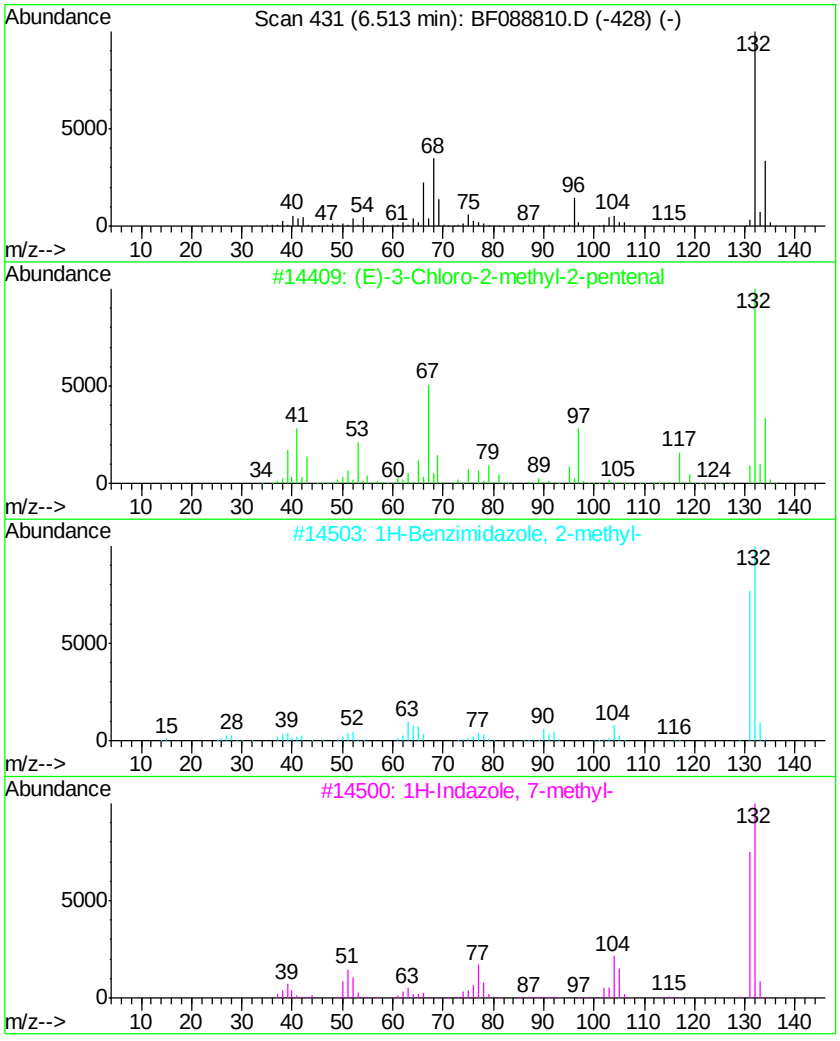
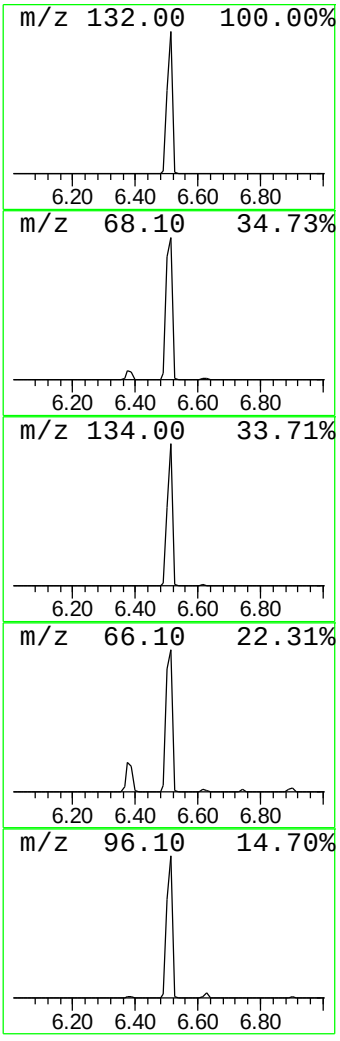
Peak Number 7 unknown6.51 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	65.92 ng	1593430	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
3	1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	12
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Sample : H3897-10
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ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
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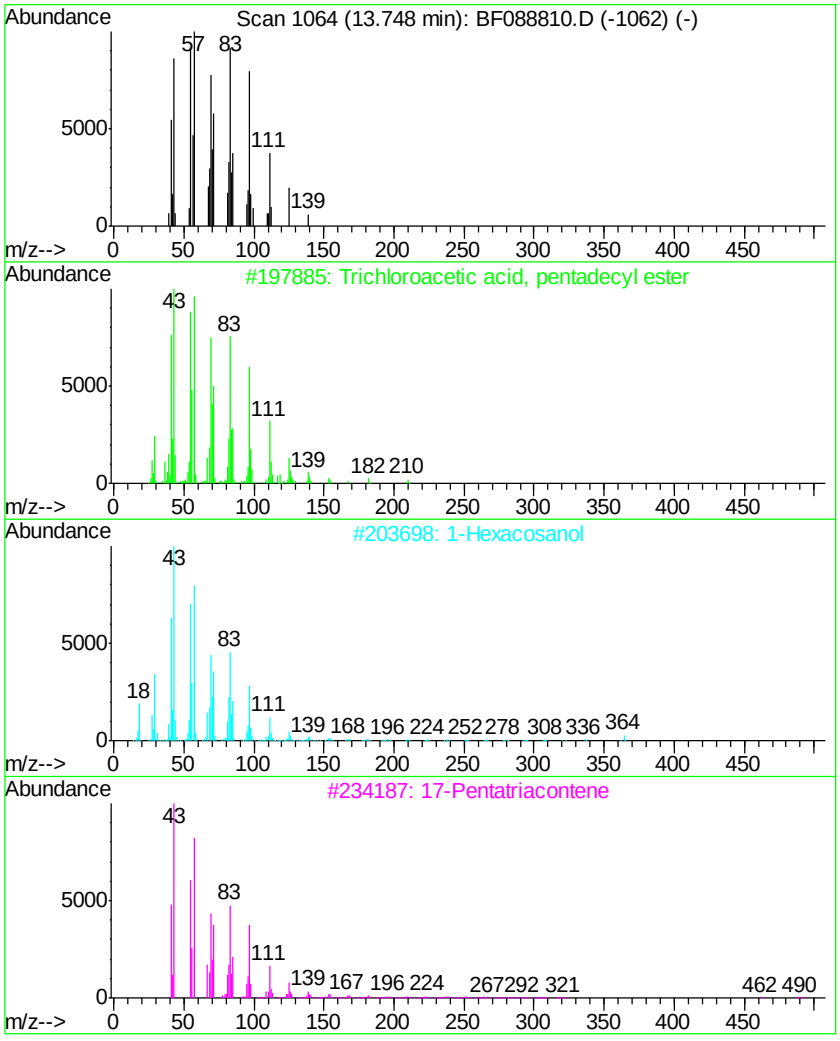
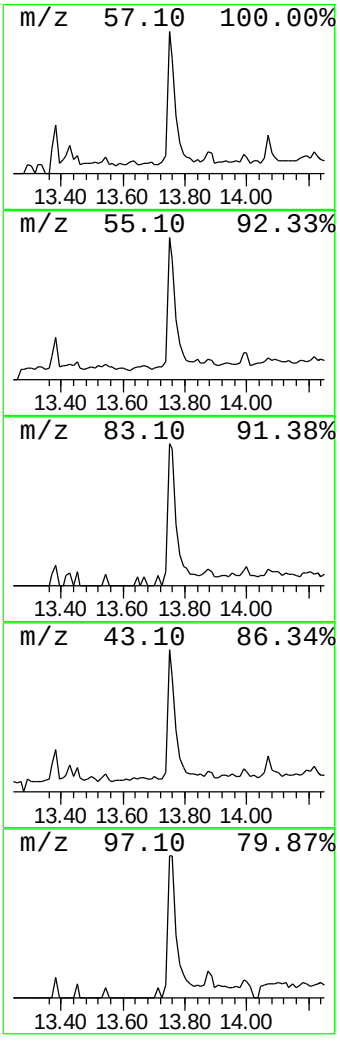
Peak Number 11 Trichloroacetic acid, penta... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	3.90 ng	103673	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
2	1-Hexacosanol	382	C26H54O	000506-52-5	91
3	17-Pentatriacontene	491	C35H70	006971-40-0	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	87
5	1-Hexadecanol	242	C16H34O	036653-82-4	83





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Acetoxyisobutyr...	4.90	4.3	ng	103133	1	6.74	483439	20.0
unknown5.24	5.24	4.5	ng	108953	1	6.74	483439	20.0
unknown5.45	5.45	2.0	ng	48444	1	6.74	483439	20.0
unknown6.51	6.51	65.9	ng	1593430	1	6.74	483439	20.0
Trichloroacetic a...	13.75	3.9	ng	103673	5	13.89	531538	20.0