LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012116\
Data File : BF084578.D
Acq On : 21 Jan 2016 12:03
Operator : SJ/UM
Sample : H1159-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SULFURCAKE

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-BF123115.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	2.441	23	31	35	rVB2	29140	114397	1.36%	0.162%
2	2.555	39	41	45	rVB	243995	297526	3.53%	0.422%
3	4.270	189	191	197	rVB	314864	456396	5.42%	0.647%
4	4.956	247	251	260	rVB	3062020	5086137	60.36%	7.214%
5	5.379	285	288	290	rBV	6011003	6198473	73.57%	8.792%
6	5.767	320	322	325	rVB	352312	326371	3.87%	0.463%
7	6.407	375	378	381	rBV	4364715	5343589	63.42%	7.579%
8	6.533	386	389	391	rBV	6626841	6279318	74.53%	8.907%
9	6.762	406	409	411	rBV	1554185	1474188	17.50%	2.091%
10	6.922	420	423	425	rVB	3905652	5267339	62.51%	7.471%
11	7.333	455	459	461	rBV	3457664	4858676	57.66%	6.892%
12	8.042	519	521	525	rBV2	2005636	2700497	32.05%	3.830%
13	8.750	581	583	586	rVB	169215	227899	2.70%	0.323%
14	8.853	589	592	594	rVB	155027	138069	1.64%	0.196%
15	9.128	612	616	618	rVB	7104434	8247884	97.89%	11.699%
16	9.790	671	674	676	rBV	1631376	2295516	27.24%	3.256%
17	9.825	676	677	679	rVB	329592	272887	3.24%	0.387%
18	9.996	690	692	695	rBV	170801	184444	2.19%	0.262%
19	10.339	720	722	724	rVB	204358	187097	2.22%	0.265%
20	10.591	740	744	746	rBV	4265554	5468194	64.90%	7.756%
21	11.276	801	804	808	rBV2	2382463	2510893	29.80%	3.562%
22	11.814	849	851	856	rBV2	86564	140729	1.67%	0.200%
23	12.876	940	944	946	rBV	6177147	8425756	100.00%	11.951%
24	13.917	1032	1035	1037	rBV	1485174	2102944	24.96%	2.983%
25	15.311	1154	1157	1159	rBV	1200557	1570915	18.64%	2.228%
26	15.608	1174	1183	1189	rBV3	70832	324453	3.85%	0.460%

Sum of corrected areas: 70500587

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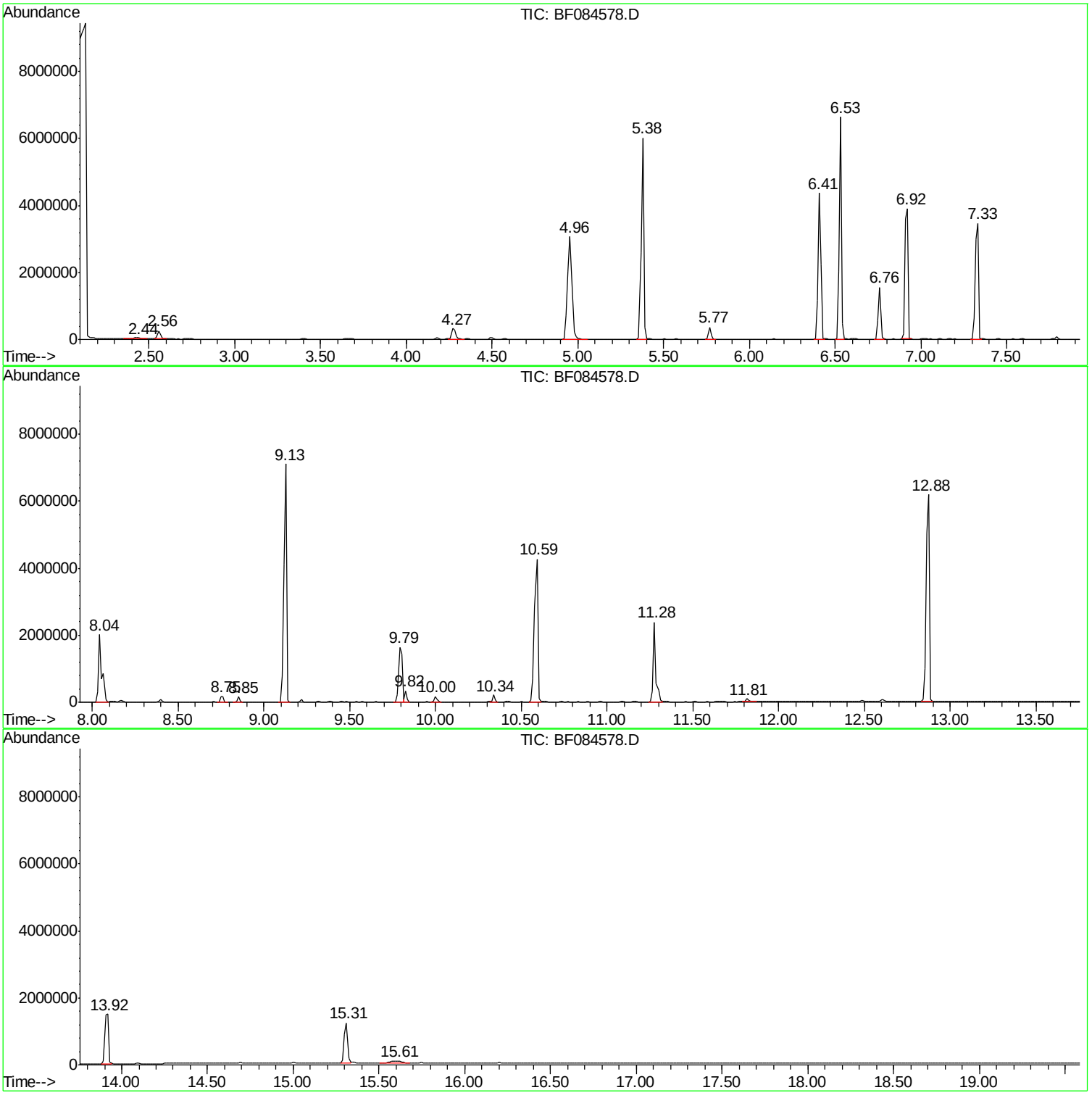
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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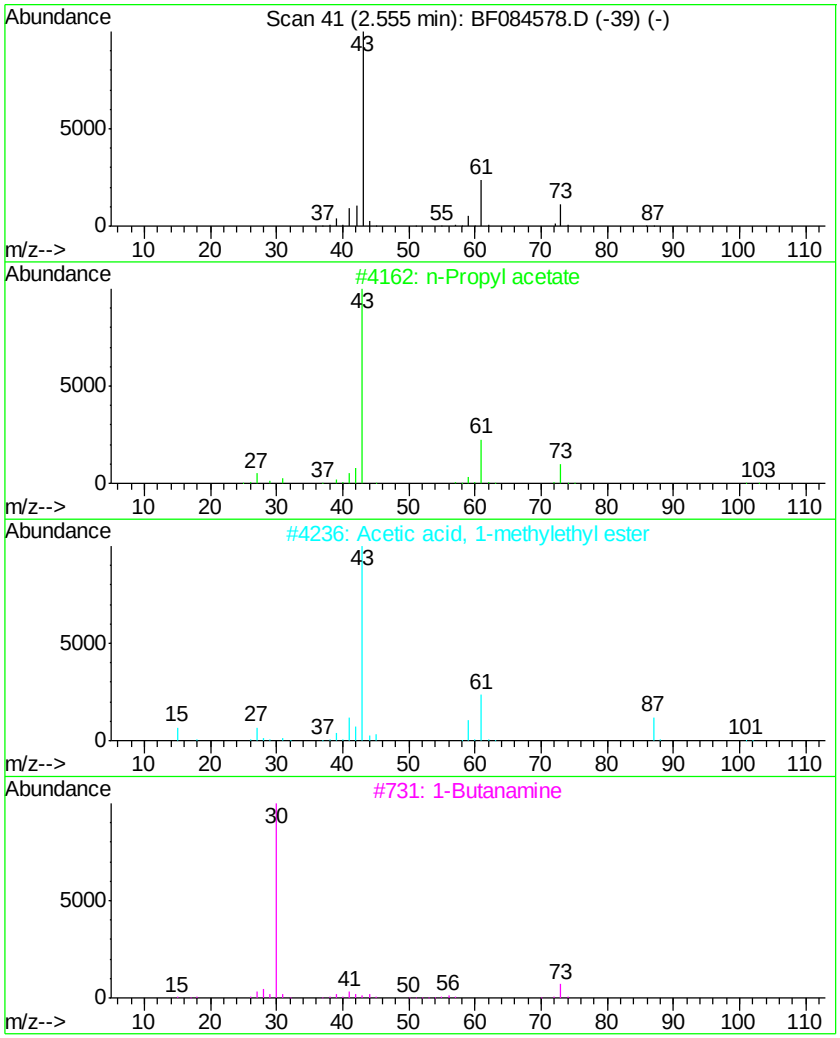
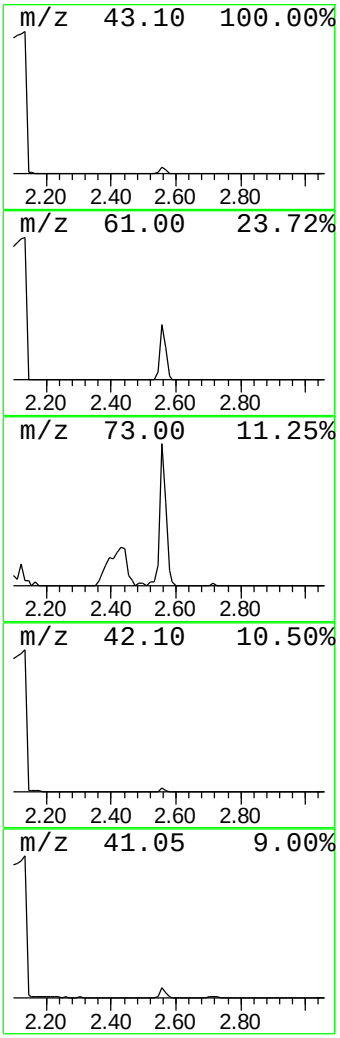
Peak Number 1 n-Propyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.56	4.04 ng	297526	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	78
2	Acetic acid, 1-methylethyl ester	102	C5H10O2	000108-21-4	36
3	1-Butanamine	73	C4H11N	000109-73-9	7
4	Isobutylamine	73	C4H11N	000078-81-9	7
5	Hydrogen azide	43	HN3	007782-79-8	4





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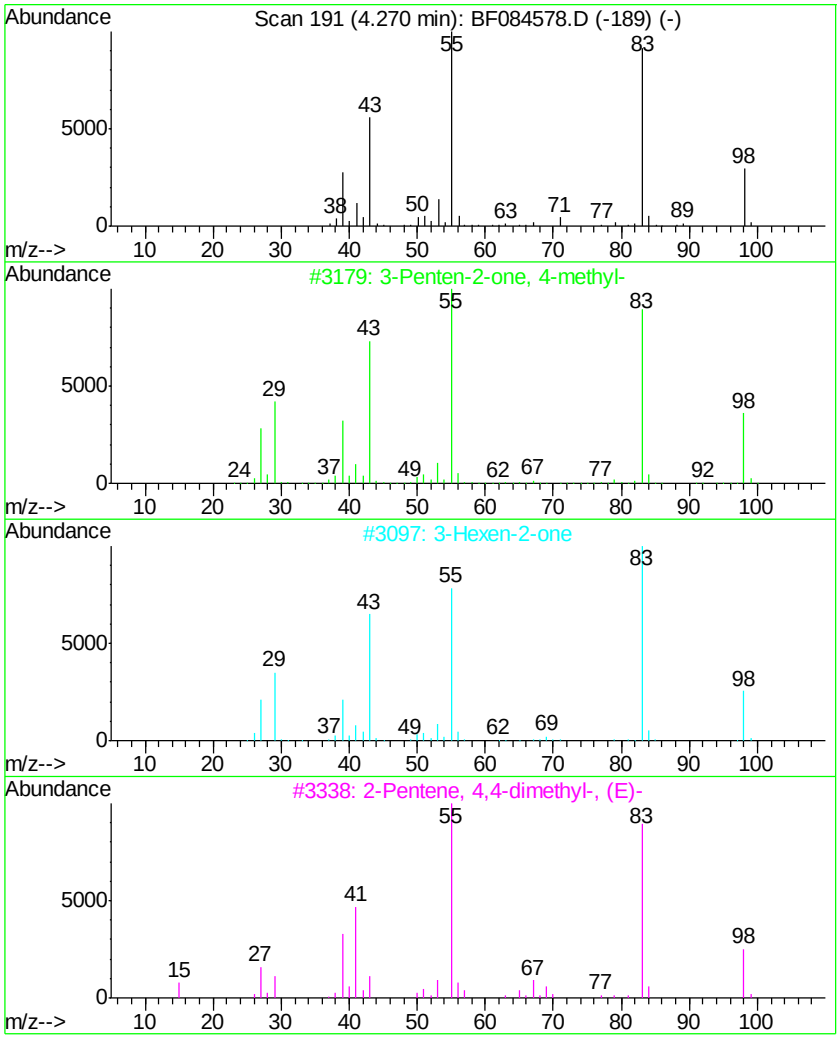
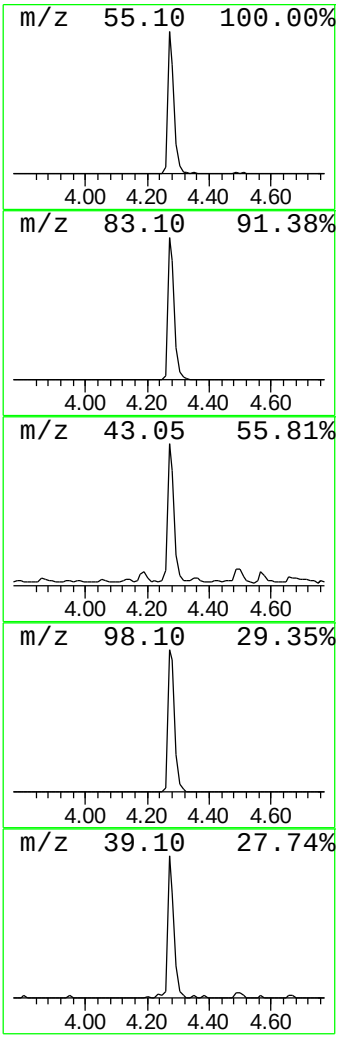
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.27	6.19 ng	456396	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	93
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	78





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ClientSampleId : SULFURCAKE

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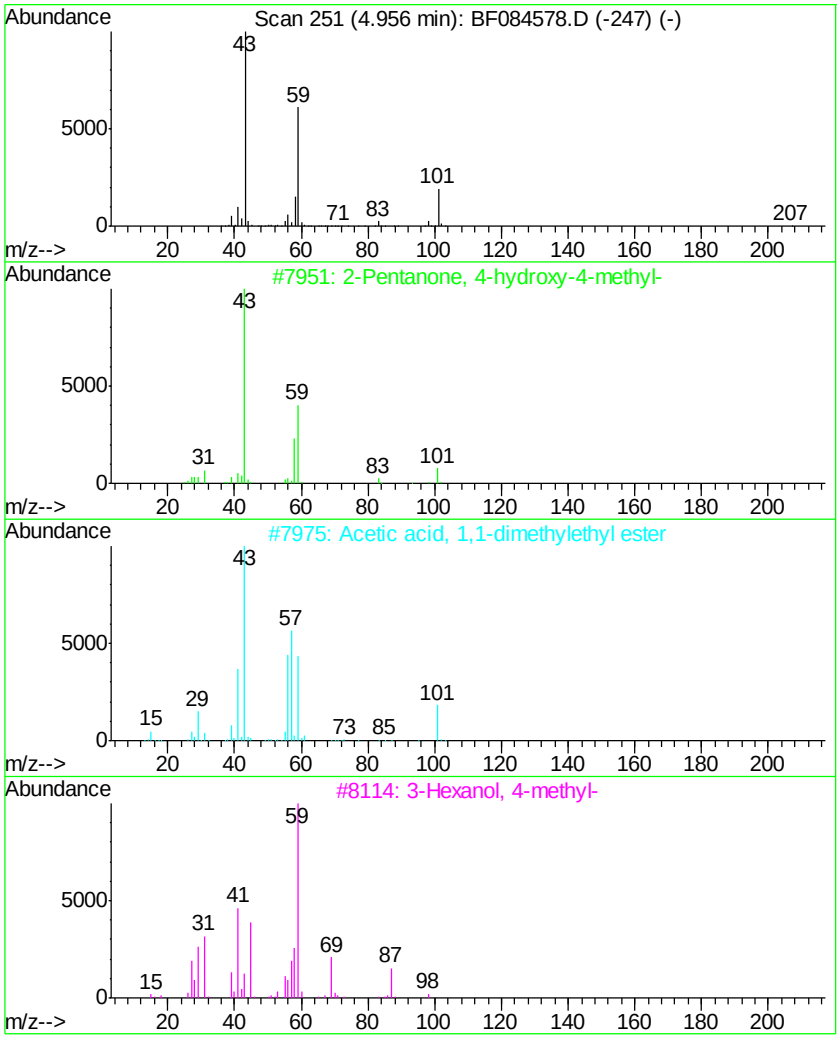
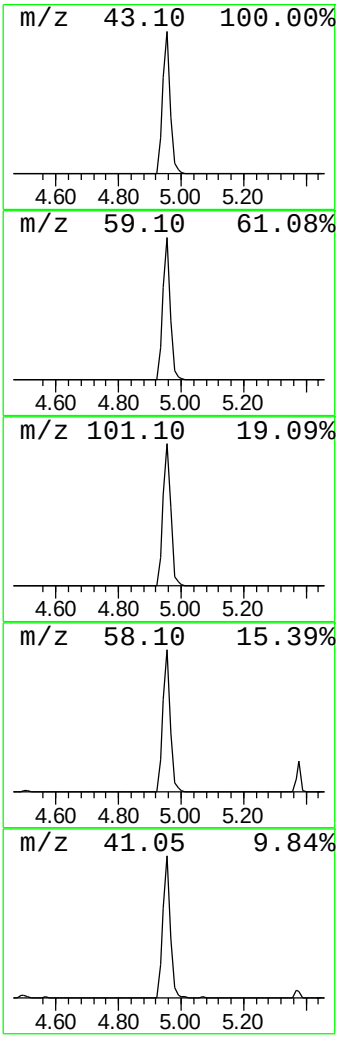
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	69.00 ng	5086140	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





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Instrument : BNA_F
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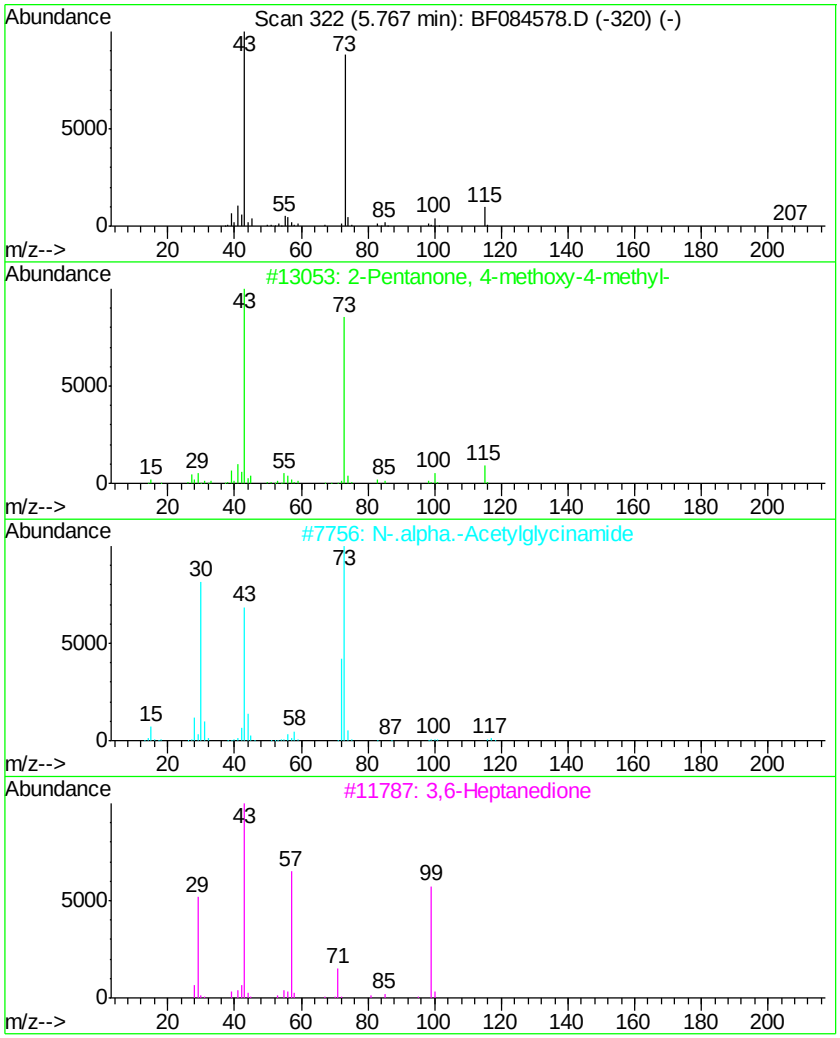
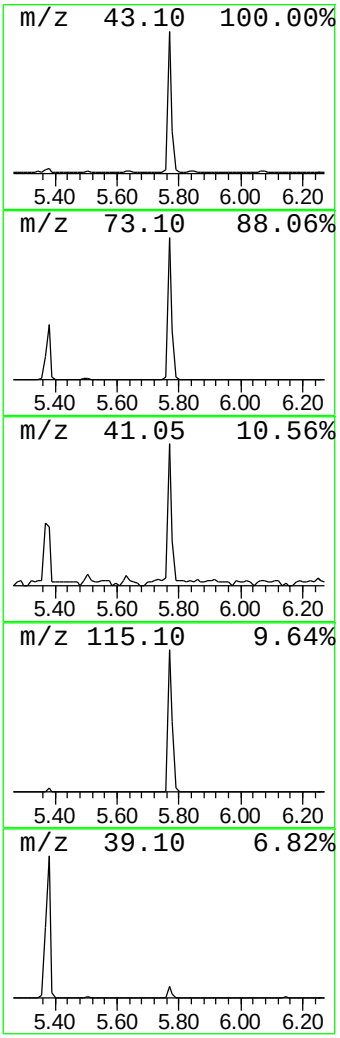
Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.77	4.43 ng	326371	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	38
3	3,6-Heptanedione	128	C7H12O2	001703-51-1	17
4	N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	10
5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	10





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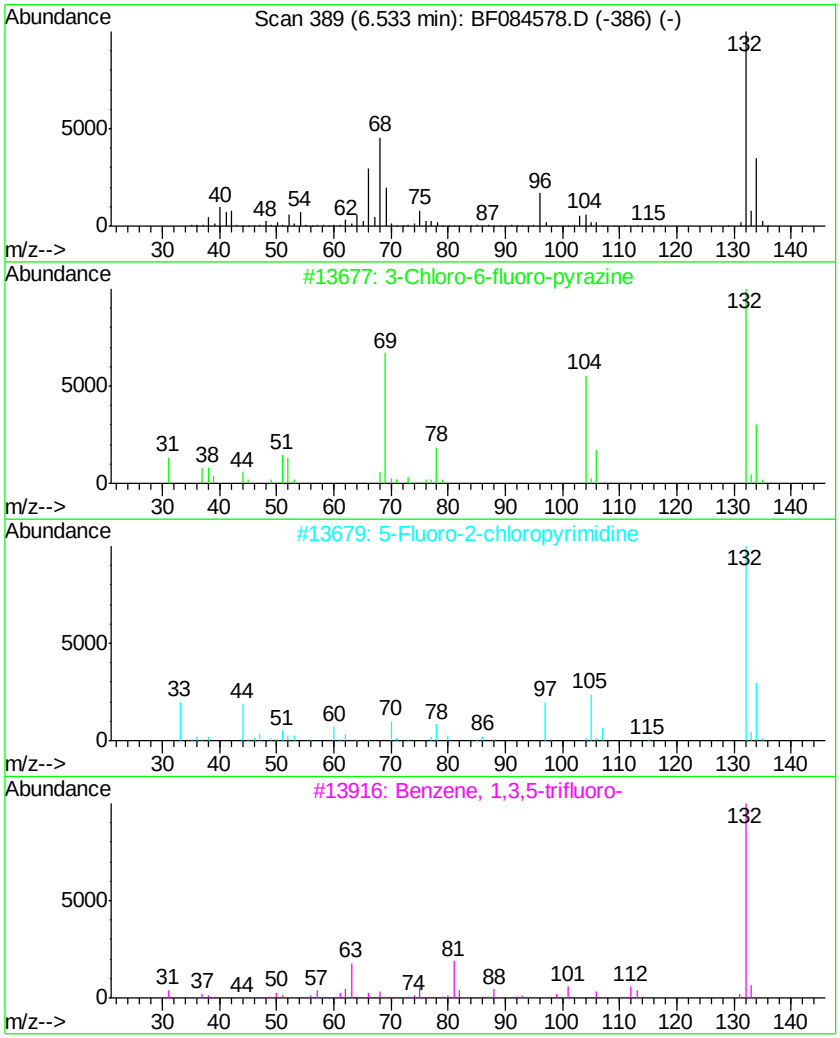
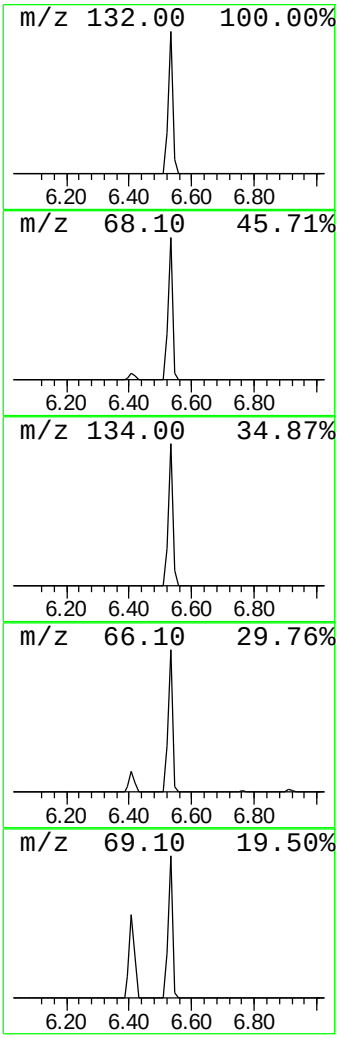
Peak Number 5 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	85.19 ng	6279320	1,4-Dichlorobenzene-d4	6.76

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	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	14
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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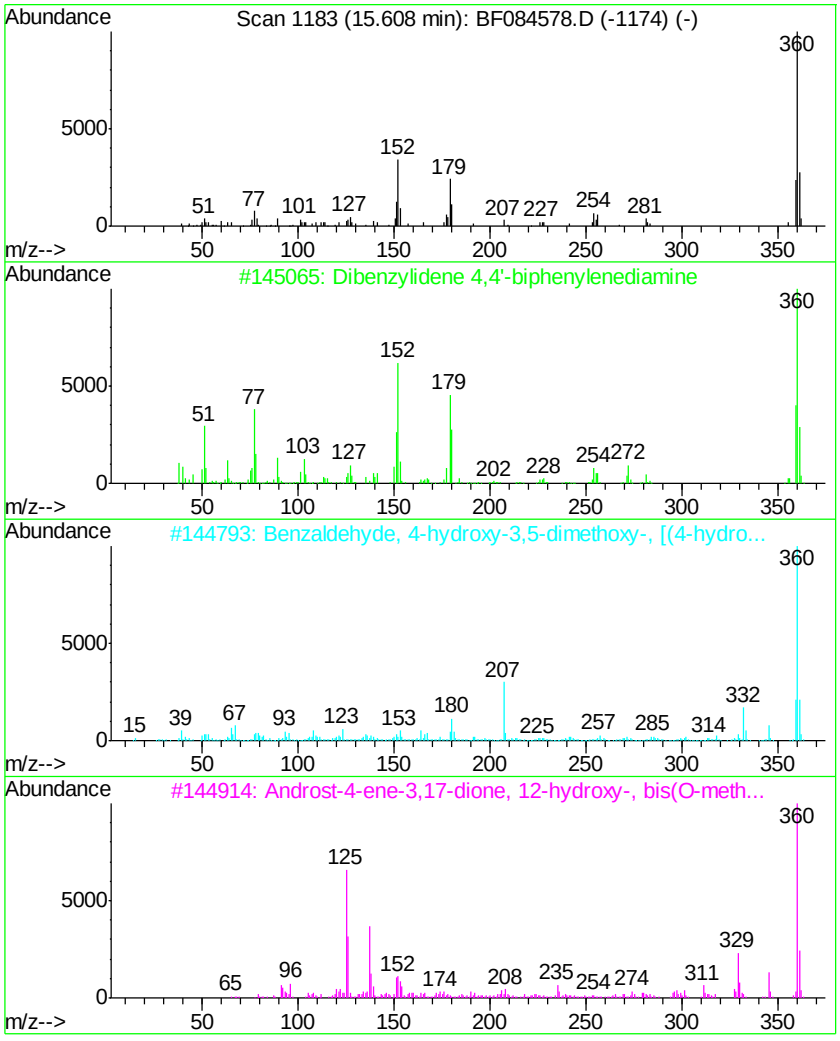
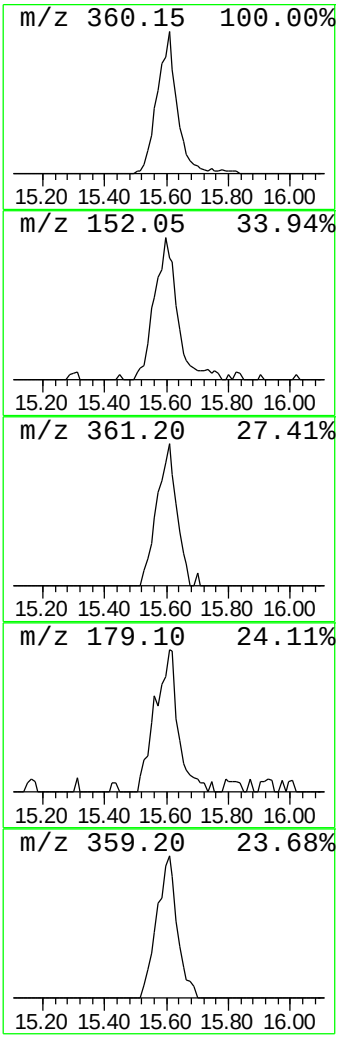
Peak Number 7 Dibenzylidene 4,4'-biphenyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.61	4.13 ng	324453	Perylene-d12	15.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	93
2	Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	53
3	Androst-4-ene-3,17-dione, 12-hyd...	360	C21H32N2O3	069688-31-9	50
4	1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13BO6	1000150-23-7	50
5	1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	50





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	2.56	4.0	ng	297526	1	6.76	1474190	20.0
3-Penten-2-one, 4...	4.27	6.2	ng	456396	1	6.76	1474190	20.0
2-Pentanone, 4-hy...	4.96	69.0	ng	5086140	1	6.76	1474190	20.0
2-Pentanone, 4-me...	5.77	4.4	ng	326371	1	6.76	1474190	20.0
unknown6.53	6.53	85.2	ng	6279320	1	6.76	1474190	20.0
Dibenzylidene 4,4...	15.61	4.1	ng	324453	6	15.31	1570920	20.0