LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011116\
Data File : BF084388.D
Acq On : 11 Jan 2016 19:12
Operator : SJ/UM
Sample : H1065-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-14

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	5.024	256	257	266	rVB	752657	1040972	10.41%	1.382%
2	5.459	293	295	298	rBV	5416806	5081835	50.82%	6.746%
3	6.499	383	386	388	rBV	2770679	3537778	35.38%	4.697%
4	6.624	394	397	399	rBV	8727618	8109213	81.09%	10.766%
5	6.853	414	417	419	rBV	2763697	2292771	22.93%	3.044%
6	7.013	428	431	433	rVB	8740548	8298199	82.98%	11.016%
7	7.425	464	467	469	rBV	6992589	7640586	76.41%	10.143%
8	7.882	503	507	511	rBV	73962	165810	1.66%	0.220%
9	8.076	520	524	527	rVB2	74015	121440	1.21%	0.161%
10	8.145	527	530	532	rBV	2426395	2921983	29.22%	3.879%
11	8.259	537	540	544	rBV4	69010	123501	1.24%	0.164%
12	9.219	621	624	627	rBV	10380411	10000064	100.00%	13.276%
13	9.402	636	640	645	rVB6	58185	165598	1.66%	0.220%
14	9.608	656	658	660	rBV	269251	281782	2.82%	0.374%
15	9.893	681	683	686	rVB	3659830	3114495	31.14%	4.135%
16	10.111	699	702	704	rBV4	65257	113875	1.14%	0.151%
17	10.328	718	721	722	rBV2	150444	186163	1.86%	0.247%
18	10.385	722	726	730	rVB5	141286	335732	3.36%	0.446%
19	10.625	745	747	749	rBV	426695	532046	5.32%	0.706%
20	10.682	749	752	755	rBV	5311856	6243924	62.44%	8.289%
21	10.796	760	762	767	rVB2	183290	307317	3.07%	0.408%
22	11.253	799	802	803	rBV	92876	109602	1.10%	0.146%
23	11.379	810	813	815	rBV	3109846	2732418	27.32%	3.627%
24	12.968	949	952	954	rBV	8071458	8058198	80.58%	10.698%
25	13.871	1029	1031	1038	rBV	123364	298250	2.98%	0.396%
26	14.008	1041	1043	1046	rBV	1673211	1857369	18.57%	2.466%
27	15.437	1165	1168	1171	rBV	1234346	1654696	16.55%	2.197%

Sum of corrected areas: 75325617

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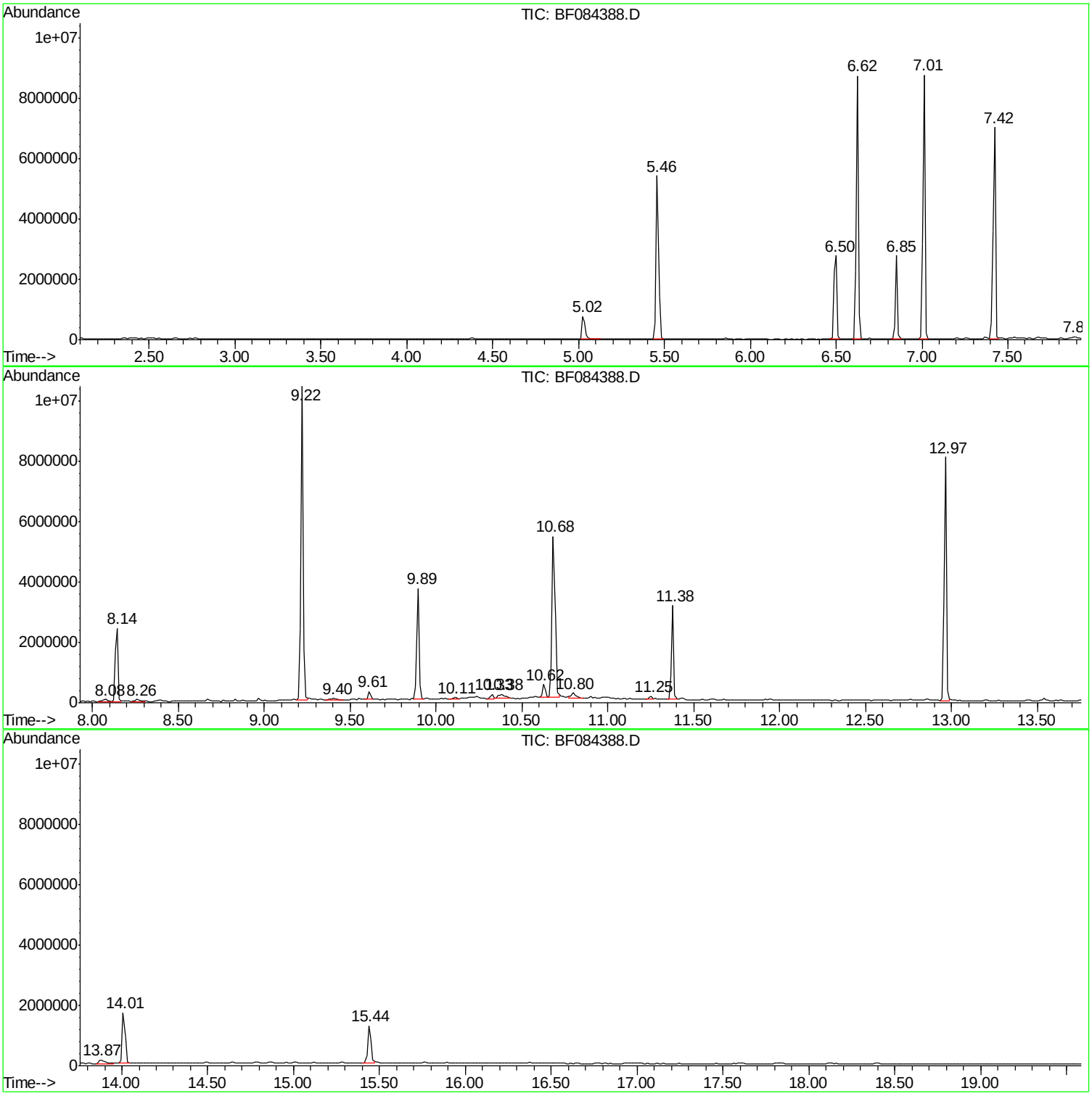
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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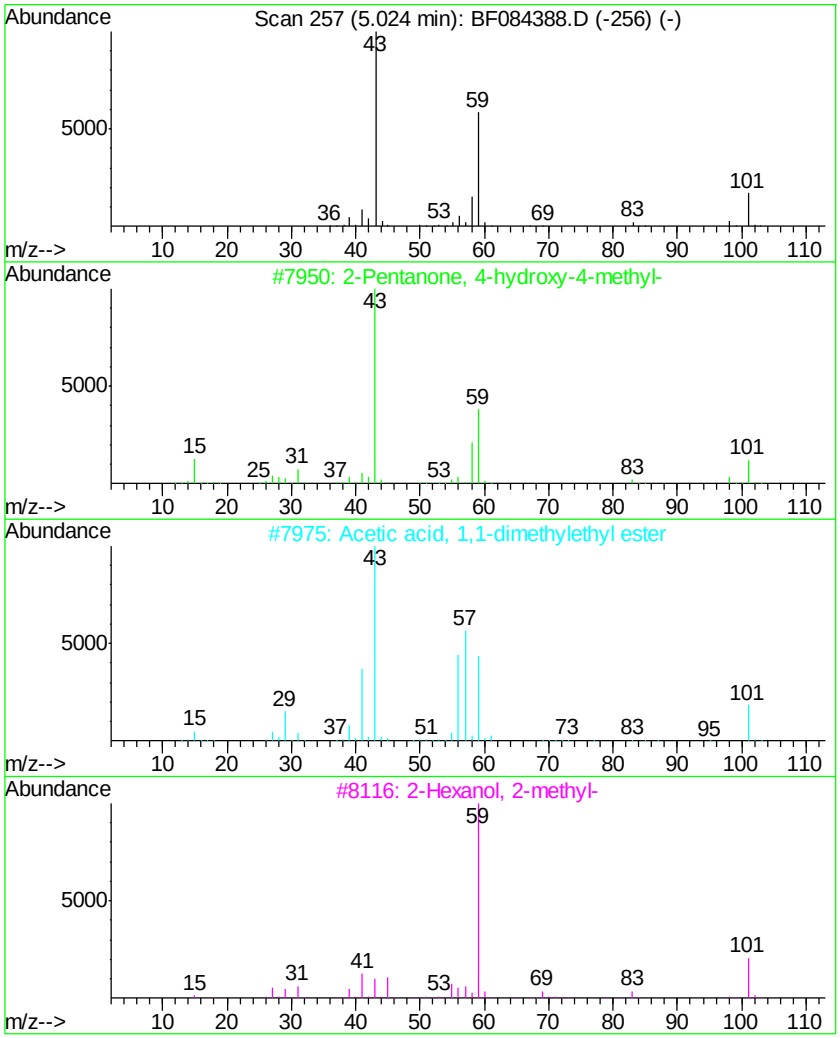
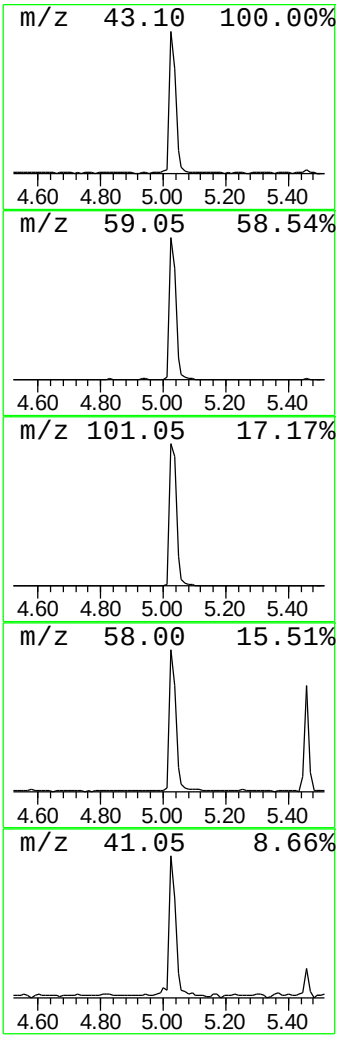
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	9.08 ng	1040970	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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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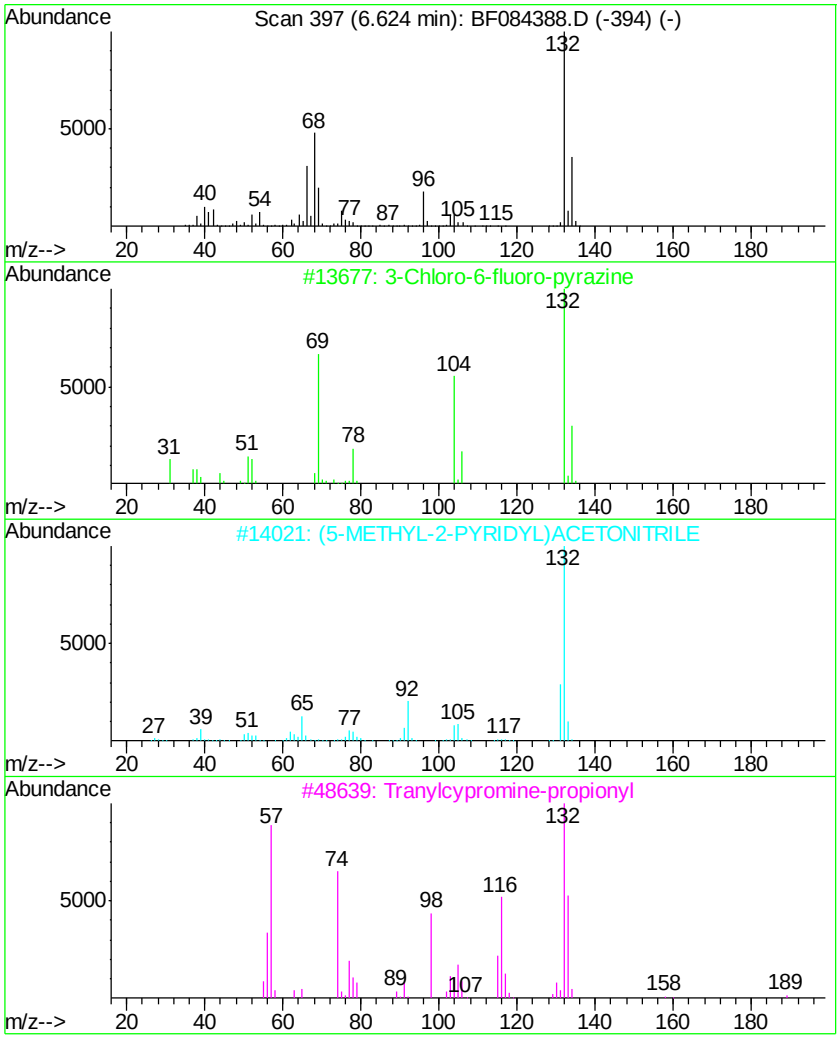
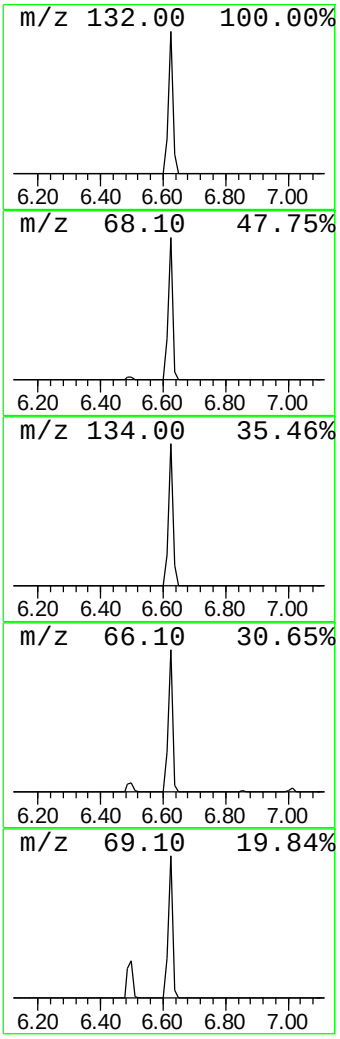
Peak Number 2 unknown6.62 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	70.74 ng	8109210	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
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	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

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Misc :
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Instrument :
BNA_F
ClientSampleId :
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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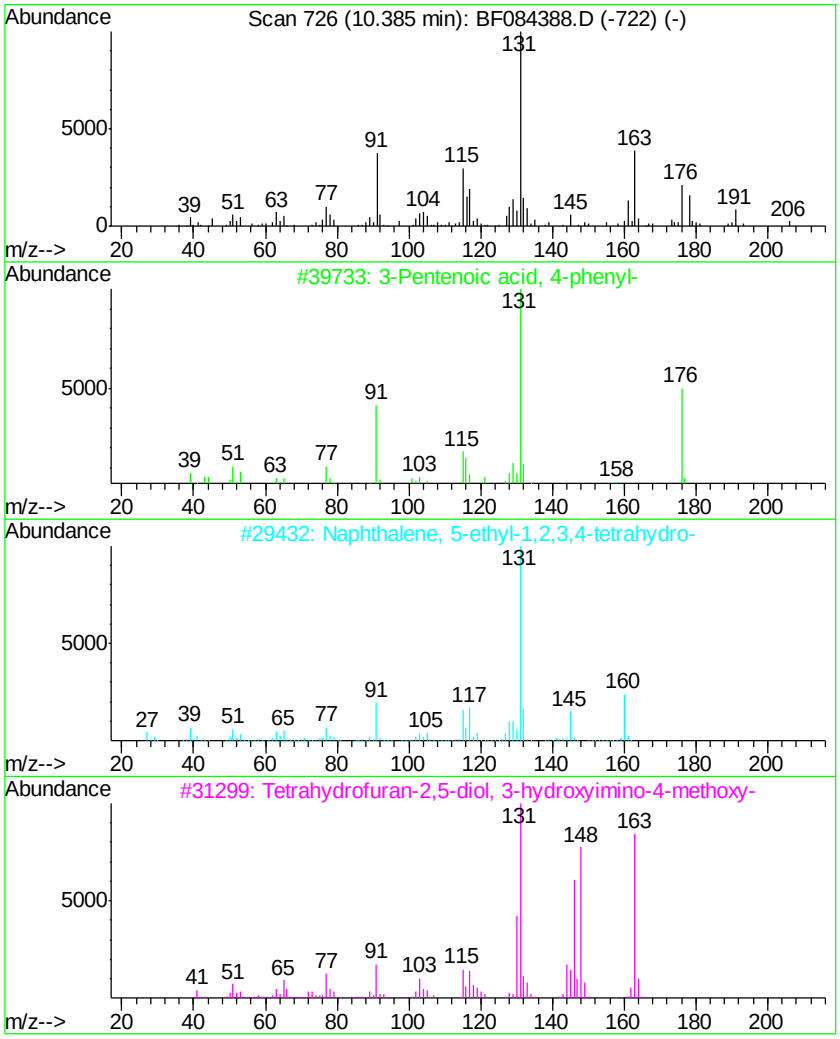
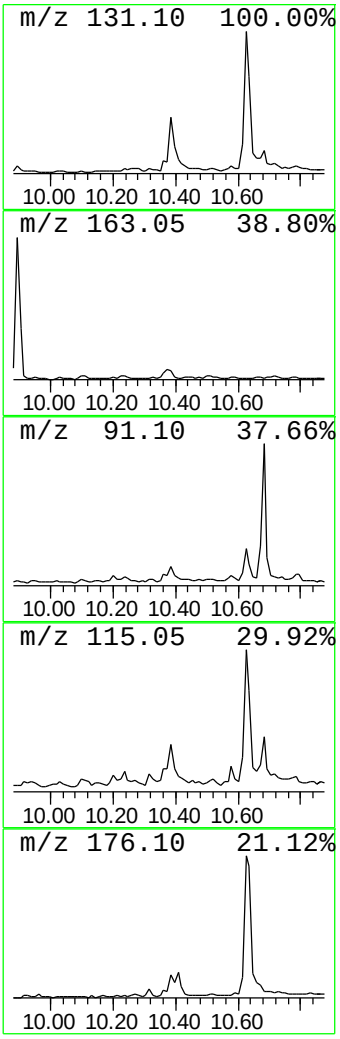
Peak Number 4 3-Pentenoic acid, 4-phenyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.38	2.16 ng	335732	Acenaphthene-d10	9.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentenoic acid, 4-phenyl-	176	C11H12O2	053774-19-9	58
2	Naphthalene, 5-ethyl-1,2,3,4-tet...	160	C12H16	042775-75-7	55
3	Tetrahydrofuran-2,5-diol, 3-hydr...	163	C5H9NO5	1000128-93-0	52
4	Benzene, (2-chloro-2-butenyl)-	166	C10H11Cl	054411-12-0	50
5	Naphthalene, 1-ethyl-1,2,3,4-tet...	160	C12H16	013556-58-6	46





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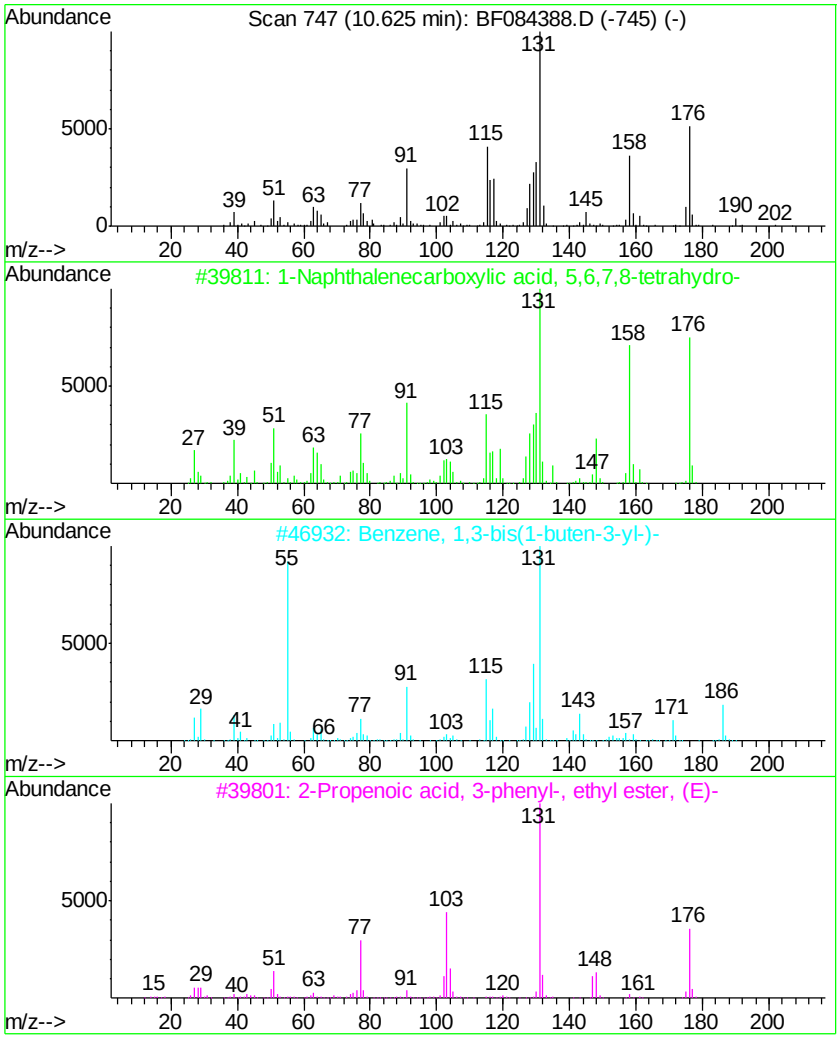
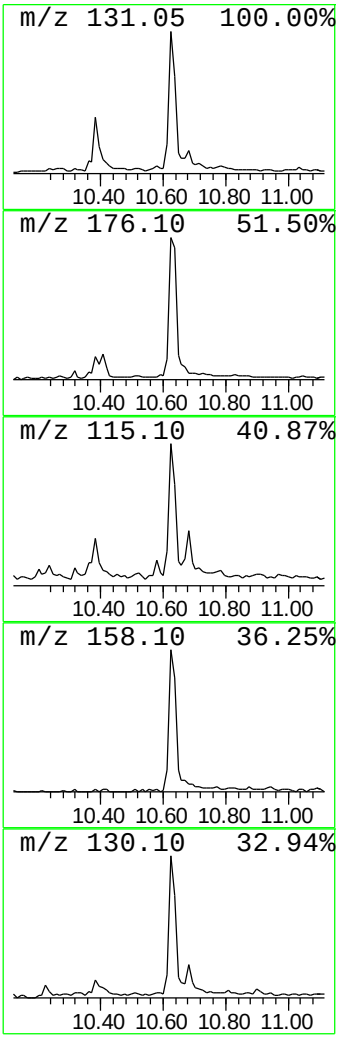
Peak Number 5 unknown10.63 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.62	3.42 ng	532046	Acenaphthene-d10	9.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Naphthalenecarboxylic acid, 5,...	176	C11H12O2	004242-18-6	43
2	Benzene, 1,3-bis(1-buten-3-yl-)-	186	C14H18	158117-62-5	38
3	2-Propenoic acid, 3-phenyl-, eth...	176	C11H12O2	004192-77-2	35
4	Cinnamic acid, .alpha.,.beta.-di...	176	C11H12O2	1000151-56-4	32
5	4,5-Diphenylocta-1,7-diene(meso)	262	C20H22	1000215-92-7	27





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BNA_F
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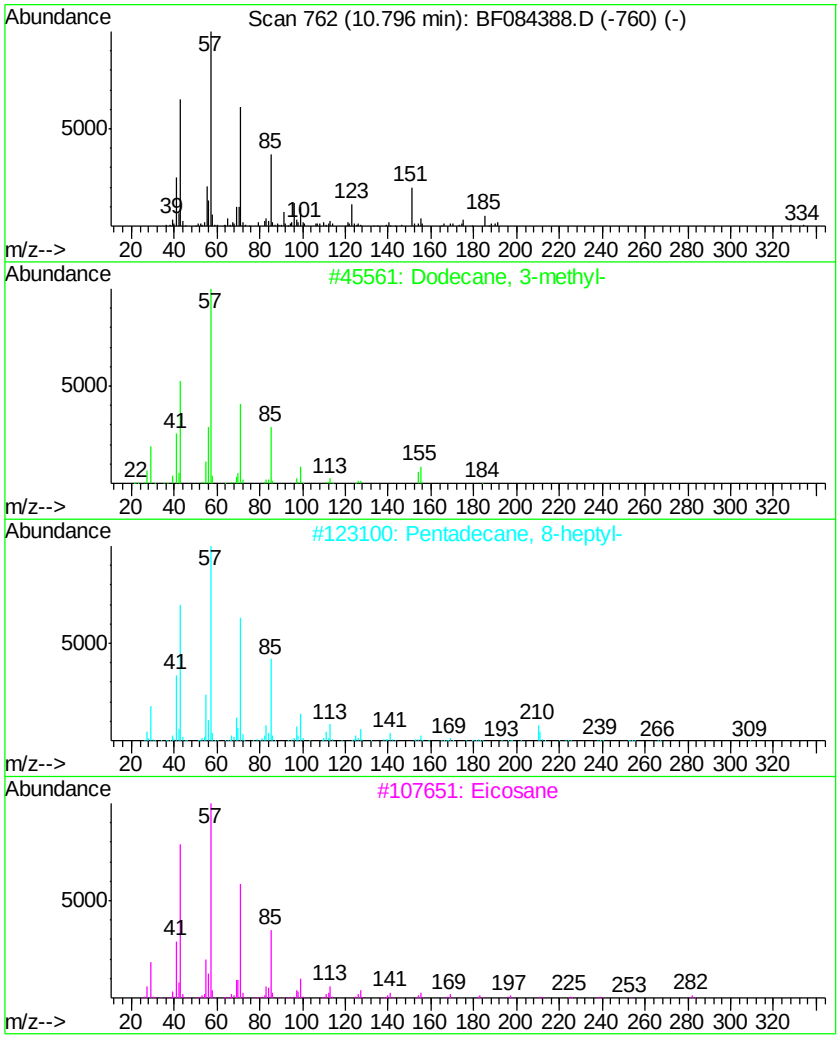
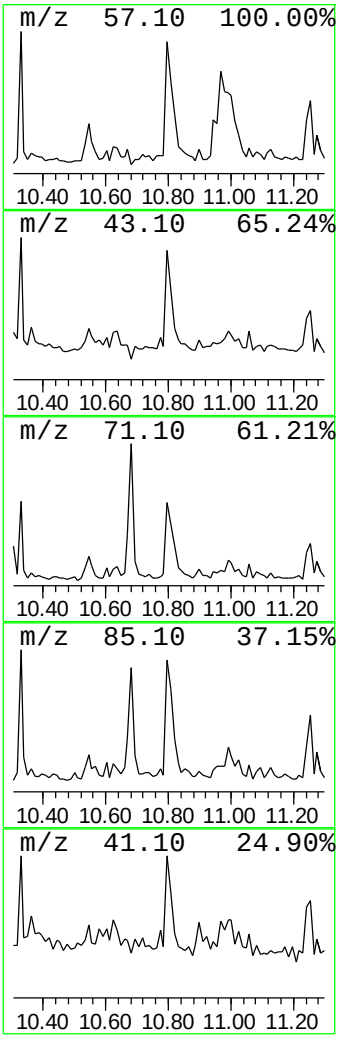
Peak Number 6 Dodecane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	2.25 ng	307317	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 3-methyl-	184	C13H28	017312-57-1	50
2	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	50
3	Eicosane	282	C20H42	000112-95-8	50
4	Decane, 3-methyl-	156	C11H24	013151-34-3	43
5	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	43





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BNA_F
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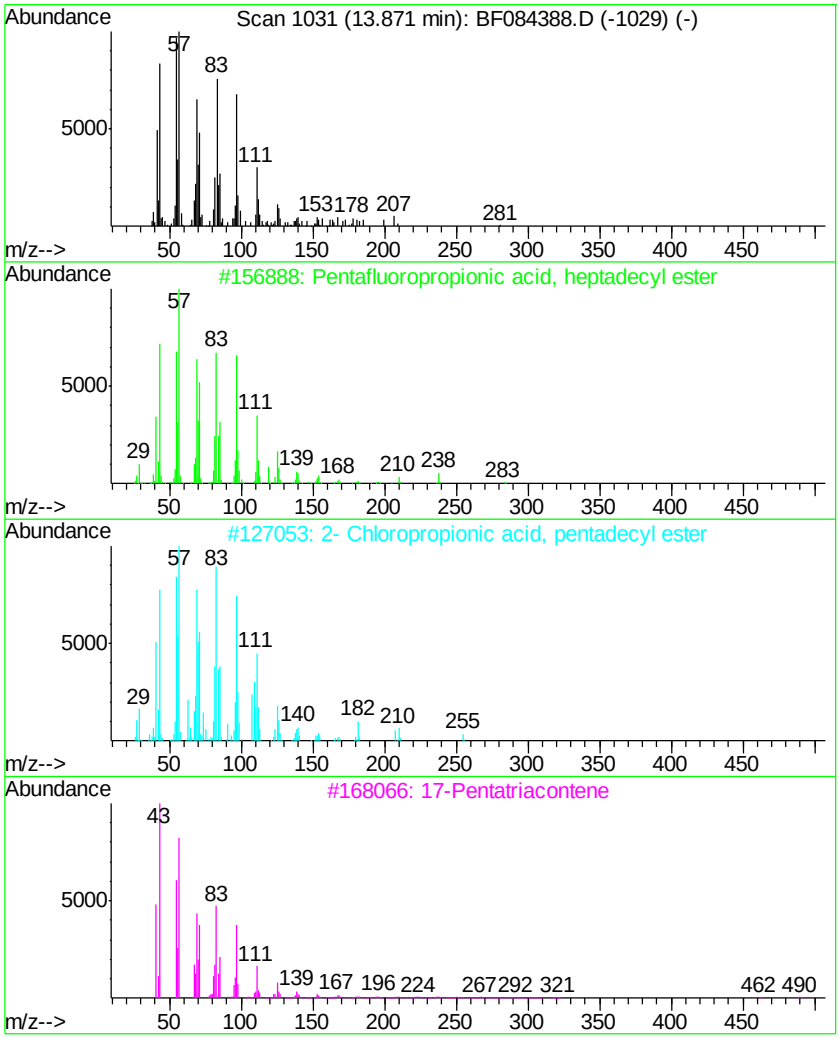
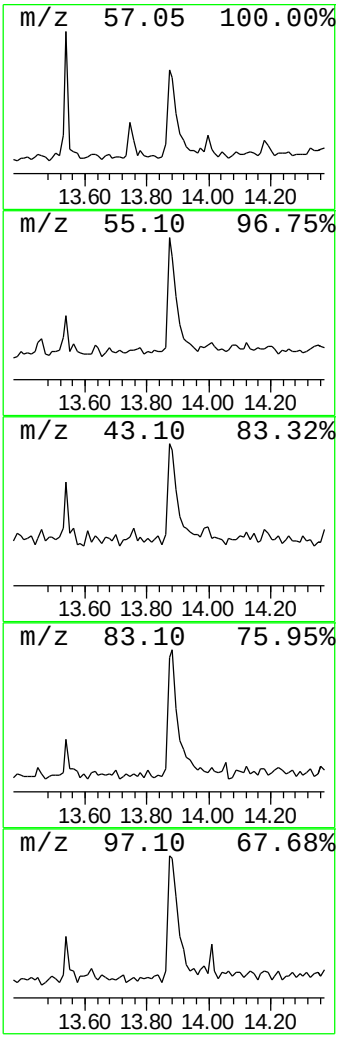
Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	3.21 ng	298250	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	94
2	2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	91
3	17-Pentatriacontene	491	C35H70	006971-40-0	91
4	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	87
5	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	87





Tentatively Identified Compound (LSC) summary

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	5.02	9.1	ng	1040970	1	6.85	2292770	20.0
unknown6.62	6.62	70.7	ng	8109210	1	6.85	2292770	20.0
3-Pentenoic acid,...	10.38	2.2	ng	335732	3	9.89	3114500	20.0
unknown10.63	10.62	3.4	ng	532046	3	9.89	3114500	20.0
Dodecane, 3-methyl-	10.80	2.3	ng	307317	4	11.38	2732420	20.0
Pentafluoropropio...	13.87	3.2	ng	298250	5	14.01	1857370	20.0