LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF093017\
Data File : BF098961.D
Acq On : 30 Sep 2017 14:31
Operator : SJ/JU
Sample : I5530-01 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LB-31(0-0.5)

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-BF092317.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	2.199	16	19	32	rVB2	46903	98694	7.67%	0.797%
2	5.128	514	517	524	rBV	85191	87707	6.82%	0.708%
3	5.522	580	584	594	rVB	625859	531914	41.33%	4.293%
4	6.528	751	755	760	rBV	624570	534778	41.55%	4.316%
5	6.675	777	780	784	rBV	704439	572353	44.47%	4.620%
6	6.910	817	820	824	rBV	958979	866631	67.34%	6.995%
7	7.069	843	847	850	rBV	525427	441675	34.32%	3.565%
8	7.469	911	915	918	rBV	414048	325754	25.31%	2.629%
9	8.198	1034	1039	1042	rBV	1224938	1155627	89.79%	9.327%
10	9.263	1216	1220	1229	rBV	720873	670381	52.09%	5.411%
11	9.657	1284	1287	1296	rVB	78711	72541	5.64%	0.586%
12	9.810	1310	1313	1316	rBV	30693	25004	1.94%	0.202%
13	9.869	1318	1323	1327	rVV2	14328	23295	1.81%	0.188%
14	9.951	1330	1337	1350	rVV	1378531	1286963	100.00%	10.388%
15	10.151	1366	1371	1375	rVB	16749	21504	1.67%	0.174%
16	10.357	1402	1406	1411	rVB2	26193	44640	3.47%	0.360%
17	10.498	1427	1430	1436	rVB	20629	22923	1.78%	0.185%
18	10.733	1467	1470	1477	rBV	349726	329443	25.60%	2.659%
19	10.845	1486	1489	1494	rBV3	26639	41574	3.23%	0.336%
20	11.045	1518	1523	1526	rBV6	11023	18450	1.43%	0.149%
21	11.292	1559	1565	1567	rBV2	30229	33321	2.59%	0.269%
22	11.333	1567	1572	1576	rVB3	16959	31190	2.42%	0.252%
23	11.439	1586	1590	1592	rBV	1330546	1163061	90.37%	9.387%
24	11.463	1592	1594	1597	rVV	240556	203441	15.81%	1.642%
25	11.510	1600	1602	1605	rVB	66619	52980	4.12%	0.428%
26	11.539	1605	1607	1611	rBV3	12215	13496	1.05%	0.109%
27	11.669	1626	1629	1631	rBV	15679	13774	1.07%	0.111%
28	11.716	1635	1637	1643	rVB4	15889	20377	1.58%	0.164%
29	11.768	1643	1646	1648	rBV3	12837	13906	1.08%	0.112%
30	11.939	1672	1675	1677	rBV	44247	48098	3.74%	0.388%
31	11.963	1677	1679	1682	rVB	44969	42829	3.33%	0.346%
32	12.051	1691	1694	1696	rBV2	53332	55184	4.29%	0.445%
33	12.233	1722	1725	1727	rBV	31700	25131	1.95%	0.203%
34	12.257	1727	1729	1733	rVB4	18947	20738	1.61%	0.167%

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.486	1765	1768	1771	rBV	35892	34361	2.67%	0.277%
36	12.515	1771	1773	1776	rBV3	28458	32722	2.54%	0.264%
37	12.568	1780	1782	1788	rBV5	23573	41126	3.20%	0.332%
38	12.651	1792	1796	1799	rBV	352026	294043	22.85%	2.373%
39	12.880	1829	1835	1841	rBV	311994	349070	27.12%	2.817%
40	13.015	1855	1858	1864	rVB	603320	527962	41.02%	4.261%
41	13.204	1888	1890	1894	rVB	55971	51233	3.98%	0.414%
42	13.310	1905	1908	1911	rBV2	33718	36903	2.87%	0.298%
43	14.074	2034	2038	2041	rBV2	805784	846405	65.77%	6.832%
44	14.098	2041	2042	2051	rVB	111819	103455	8.04%	0.835%
45	14.592	2123	2126	2132	rBV3	80189	102700	7.98%	0.829%
46	15.127	2214	2217	2220	rBV	115220	153168	11.90%	1.236%
47	15.504	2278	2281	2287	rVB	75233	112233	8.72%	0.906%
48	15.568	2288	2292	2302	rVB	554688	794731	61.75%	6.415%

Sum of corrected areas: 12389489

LSC Report - Integrated Chromatogram

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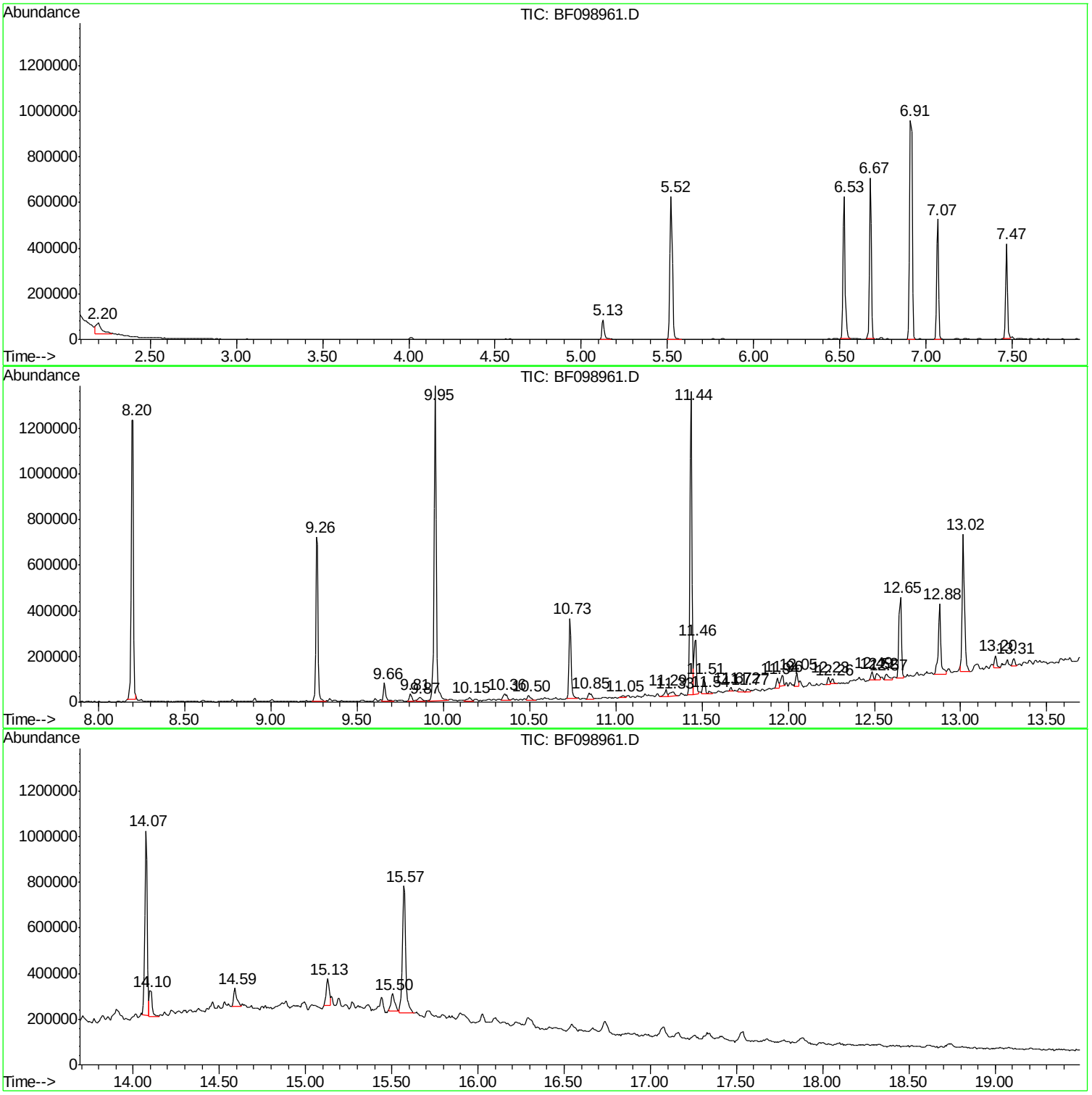
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LB-31(0-0.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF093017\
Data File : BF098961.D
Acq On : 30 Sep 2017 14:31
Operator : SJ/JU
Sample : I5530-01 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LB-31(0-0.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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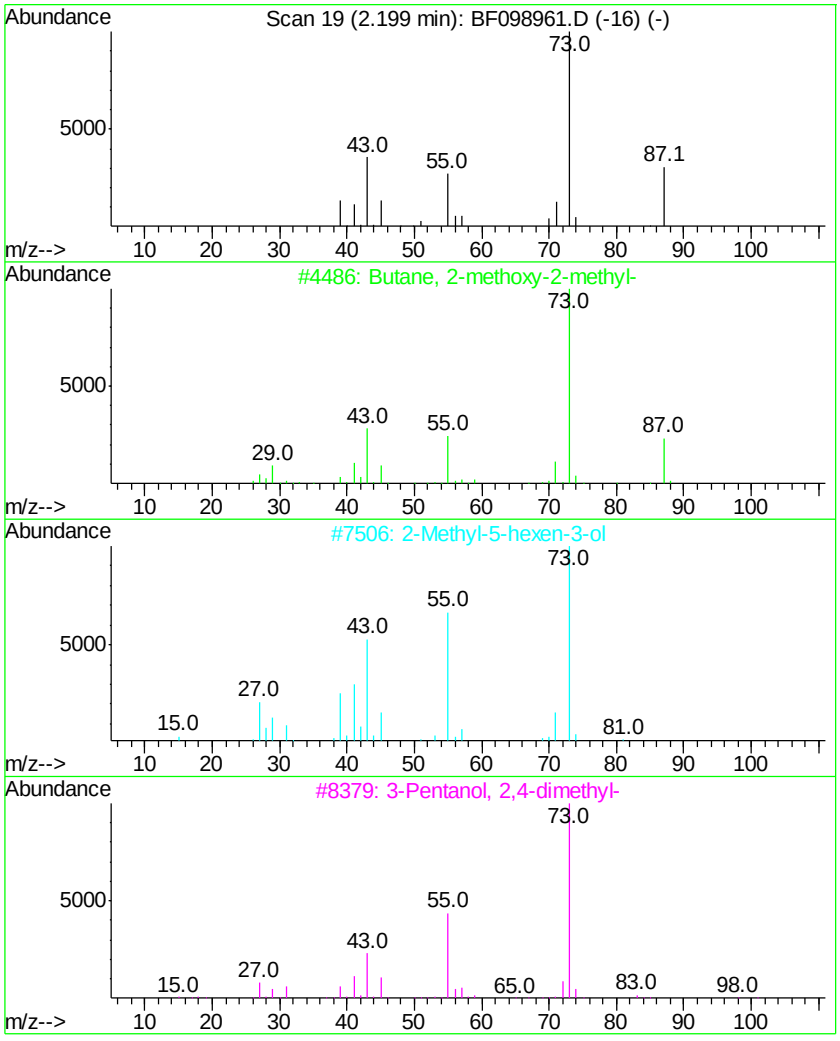
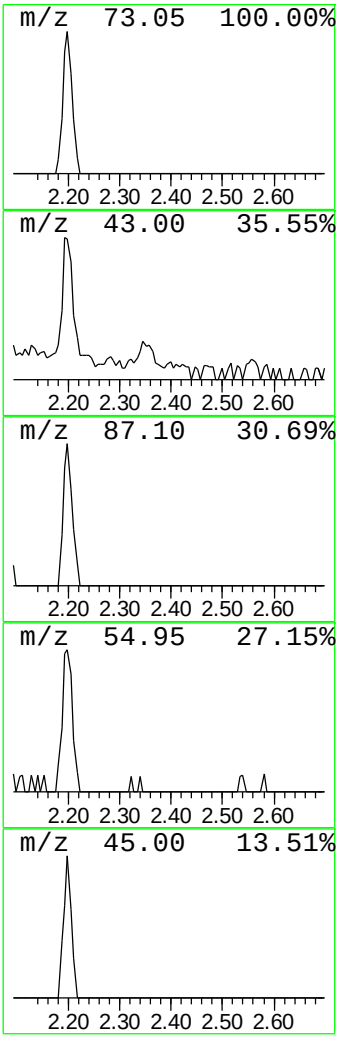
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	2.28 ng	98694	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	28
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9
4	Acetamide, N-(2-hydroxy-3-penten...	143	C7H13NO2	093393-95-4	9
5	Ethyl formate	74	C3H6O2	000109-94-4	4





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Instrument : BNA_F
ClientSampleId : LB-31(0-0.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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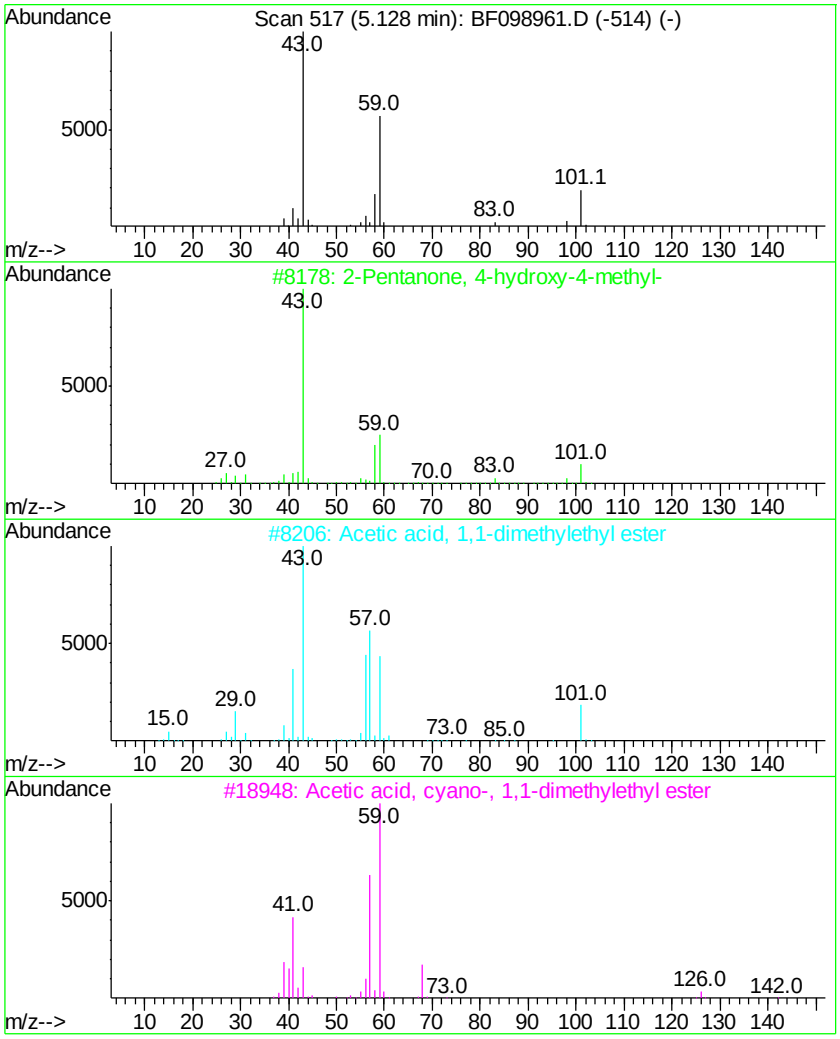
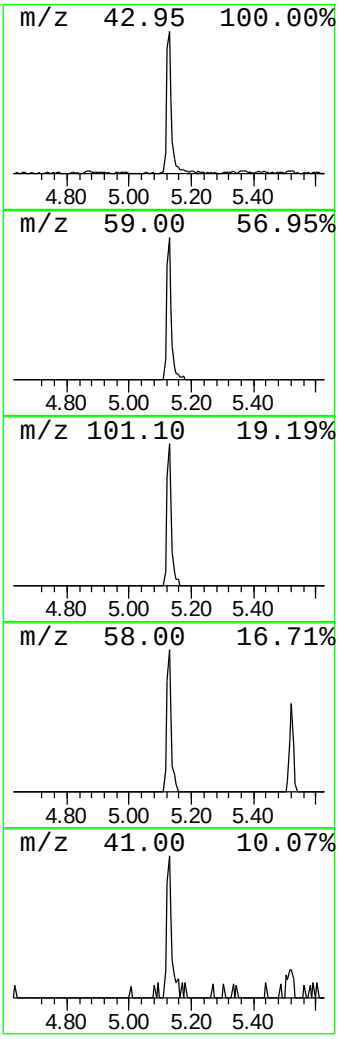
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	2.02 ng	87707	1,4-Dichlorobenzene-d4	6.92

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	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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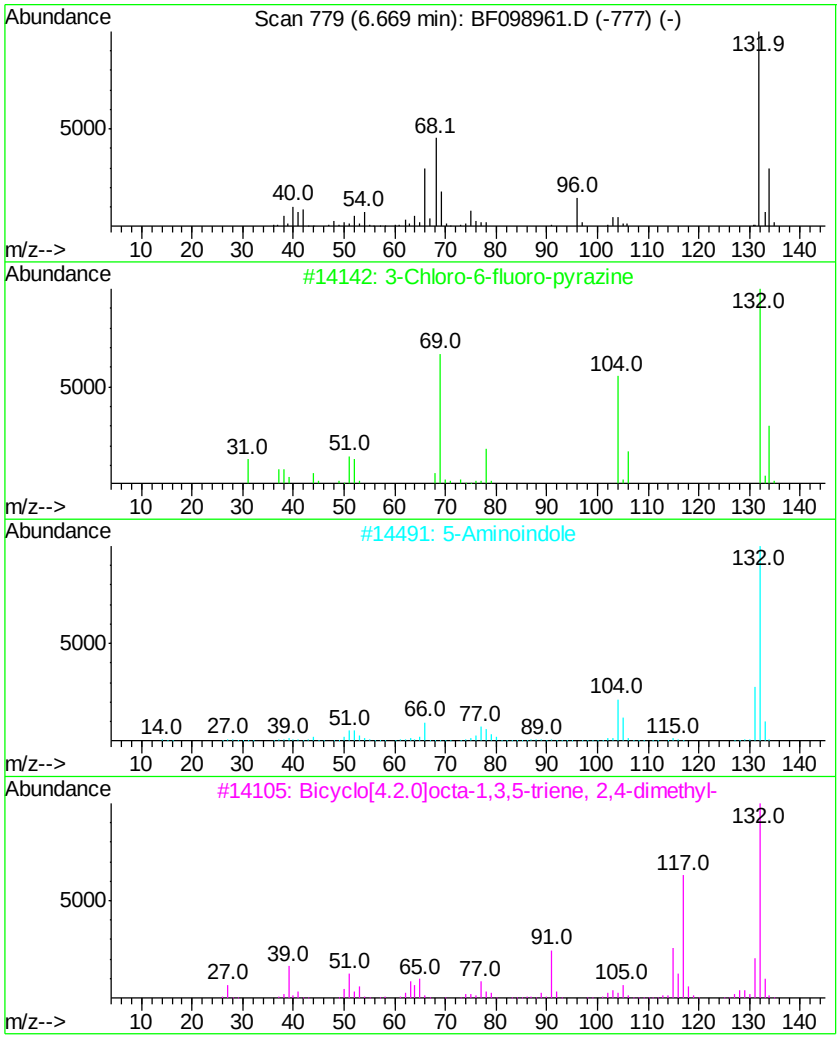
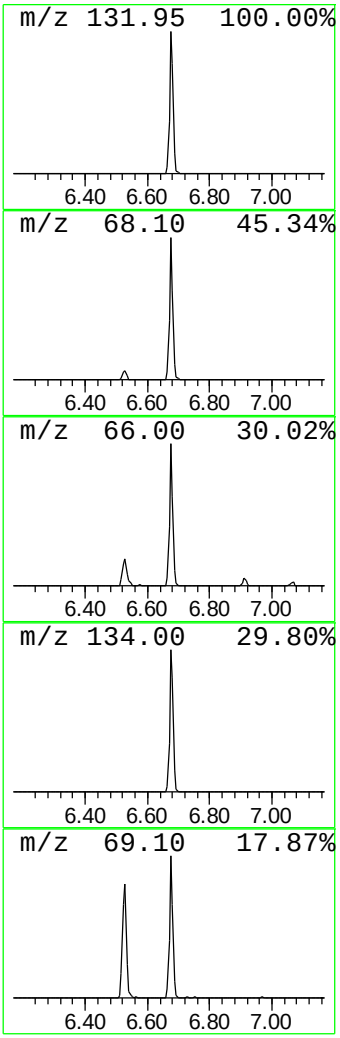
****

Peak Number 3 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	13.21 ng	572353	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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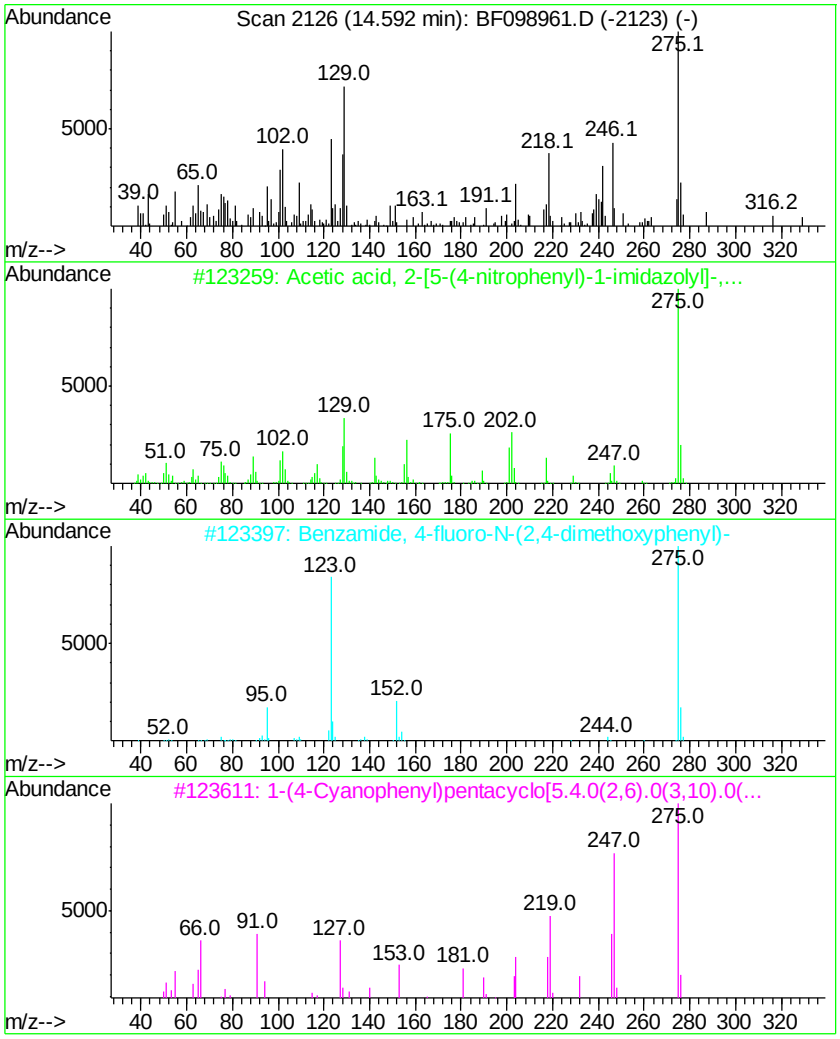
TIC Integration Parameters: LSCINT.P

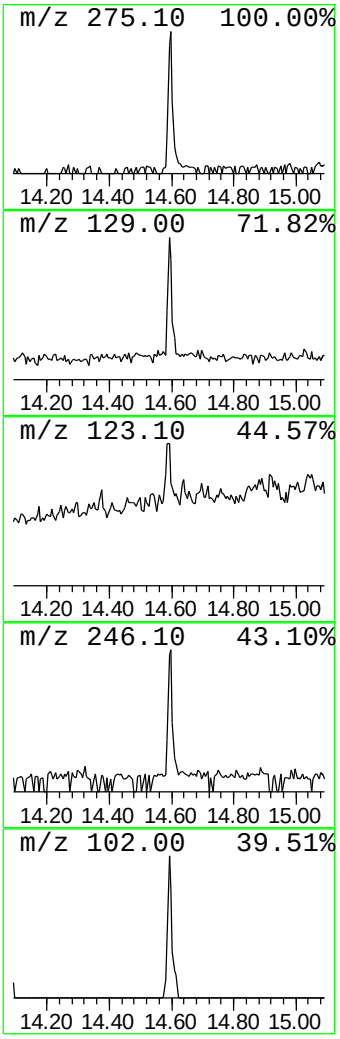
****

Peak Number 5 unknown14.59 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	2.43 ng	102700	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 2-[5-(4-nitrophenyl...	275	C13H13N3O4	351064-45-4	47
2	Benzamide, 4-fluoro-N-(2,4-dimet...	275	C15H14FNO3	1000340-32-6	35
3	1-(4-Cyanophenyl)pentacyclo[5.4....	275	C18H13NO2	118171-98-5	35
4	1-Methyl-5'-phenylspiro(indoline...	275	C17H13N3O	015970-21-5	27
5	8H-Benzo[g]-1,3-benzodioxolo[6,5...	275	C17H9NO3	000475-75-2	27





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.20	2.3	ng	98694	1	6.92	866631	20.0
2-Pentanone, 4-hy...	5.13	2.0	ng	87707	1	6.92	866631	20.0
unknown6.67	6.67	13.2	ng	572353	1	6.92	866631	20.0
unknown14.59	14.59	2.4	ng	102700	5	14.07	846405	20.0