LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085266.D
Acq On : 8 Mar 2016 20:13
Operator : UM/SJ
Sample : H1684-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RW-48-S2 GRID 3

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-BF030316.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	2.858	47	50	55	rVB	95105	146177	3.04%	0.366%
2	4.538	195	197	202	rBV	219611	309212	6.43%	0.775%
3	5.167	249	252	256	rBV	845608	1207617	25.12%	3.026%
4	5.567	283	287	290	rBV	2548885	3861848	80.32%	9.678%
5	6.481	366	367	369	rBV	77619	75956	1.58%	0.190%
6	6.584	373	376	378	rVB	3237747	3269343	67.99%	8.193%
7	6.733	386	389	391	rBV	3448312	4199978	87.35%	10.526%
8	6.790	391	394	396	rVV	194300	199259	4.14%	0.499%
9	6.961	406	409	411	rBV	1050816	886589	18.44%	2.222%
10	7.019	411	414	416	rVB	85254	66315	1.38%	0.166%
11	7.122	420	423	424	rBV	3347098	3470446	72.18%	8.697%
12	7.522	455	458	460	rVB	2602901	2587634	53.82%	6.485%
13	7.979	494	498	500	rVB2	71312	89957	1.87%	0.225%
14	8.264	519	523	525	rBV2	1598364	2478479	51.55%	6.211%
15	8.310	525	527	529	rVB	57854	73082	1.52%	0.183%
16	8.950	581	583	586	rVB	161687	218313	4.54%	0.547%
17	9.053	590	592	594	rVB	96604	82182	1.71%	0.206%
18	9.327	612	616	618	rBV	3350201	4808300	100.00%	12.050%
19	10.002	672	675	677	rBV	1233360	1143961	23.79%	2.867%
20	10.790	741	744	746	rBV	2698721	2676799	55.67%	6.708%
21	11.488	802	805	807	rBV	1134407	1183401	24.61%	2.966%
22	13.076	941	944	946	rBV	3675261	4579198	95.24%	11.476%
23	14.116	1033	1035	1038	rBV	1026547	904066	18.80%	2.266%
24	15.579	1160	1163	1166	rBV	539401	699824	14.55%	1.754%
25	17.134	1297	1299	1302	rBV4	38463	95475	1.99%	0.239%
26	17.500	1328	1331	1335	rBV5	23859	59439	1.24%	0.149%
27	17.603	1336	1340	1343	rBV5	32429	51504	1.07%	0.129%
28	17.808	1355	1358	1361	rBV5	66511	127726	2.66%	0.320%
29	17.865	1361	1363	1365	rVV3	39114	81642	1.70%	0.205%
30	17.900	1365	1366	1369	rVB2	46611	56175	1.17%	0.141%
31	18.185	1388	1391	1392	rVB2	57292	78389	1.63%	0.196%
32	18.505	1417	1419	1422	rVB3	63135	80114	1.67%	0.201%
33	18.928	1454	1456	1460	rVB2	54123	53779	1.12%	0.135%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085266.D
Acq On : 8 Mar 2016 20:13
Operator : UM/SJ
Sample : H1684-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RW-48-S2 GRID 3

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-BF030316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

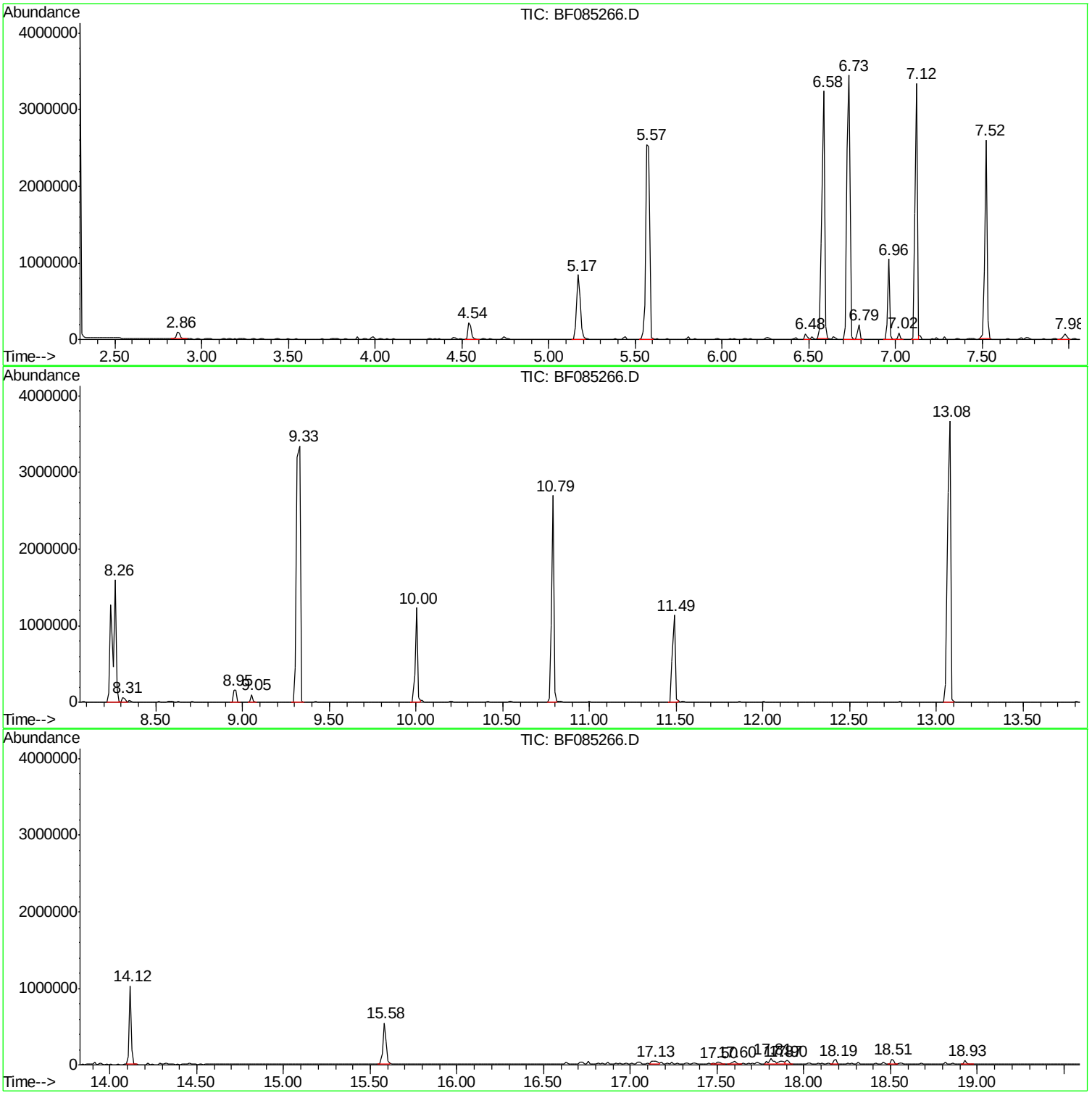
Sum of corrected areas: 39902179

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085266.D
Acq On : 8 Mar 2016 20:13
Operator : UM/SJ
Sample : H1684-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RW-48-S2 GRID 3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085266.D
Acq On : 8 Mar 2016 20:13
Operator : UM/SJ
Sample : H1684-11
Misc :
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Instrument : BNA_F
ClientSampleId : RW-48-S2 GRID 3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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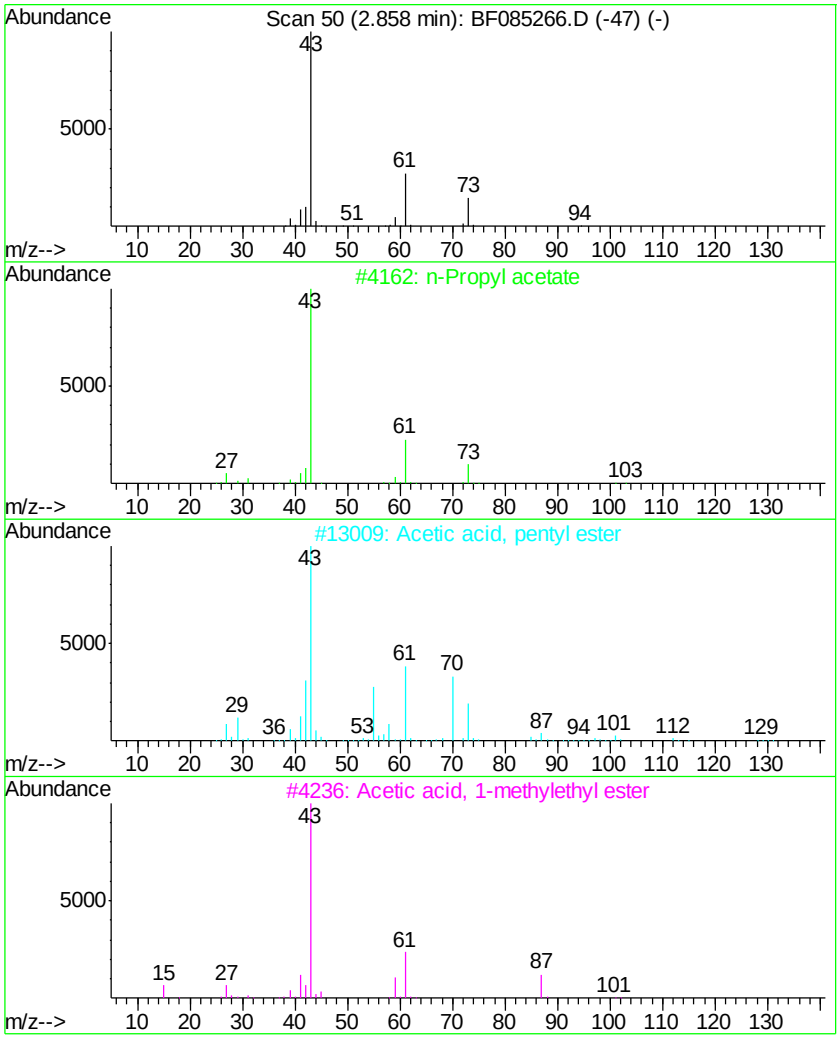
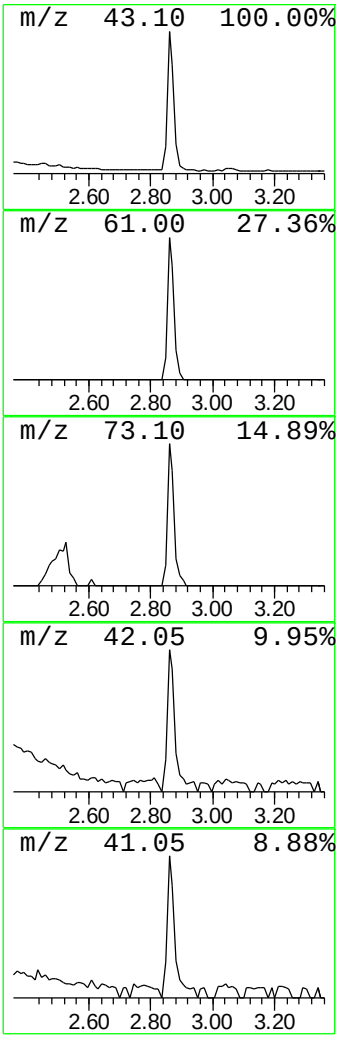
Peak Number 1 n-Propyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.86	3.30 ng	146177	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	78
2	Acetic acid, pentyl ester	130	C7H14O2	000628-63-7	9
3	Acetic acid, 1-methylethyl ester	102	C5H10O2	000108-21-4	9
4	1-Propanol, 3-chloro-, acetate	136	C5H9ClO2	000628-09-1	9
5	Acetohydroxamic Acid	75	C2H5NO2	000546-88-3	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085266.D
Acq On : 8 Mar 2016 20:13
Operator : UM/SJ
Sample : H1684-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RW-48-S2 GRID 3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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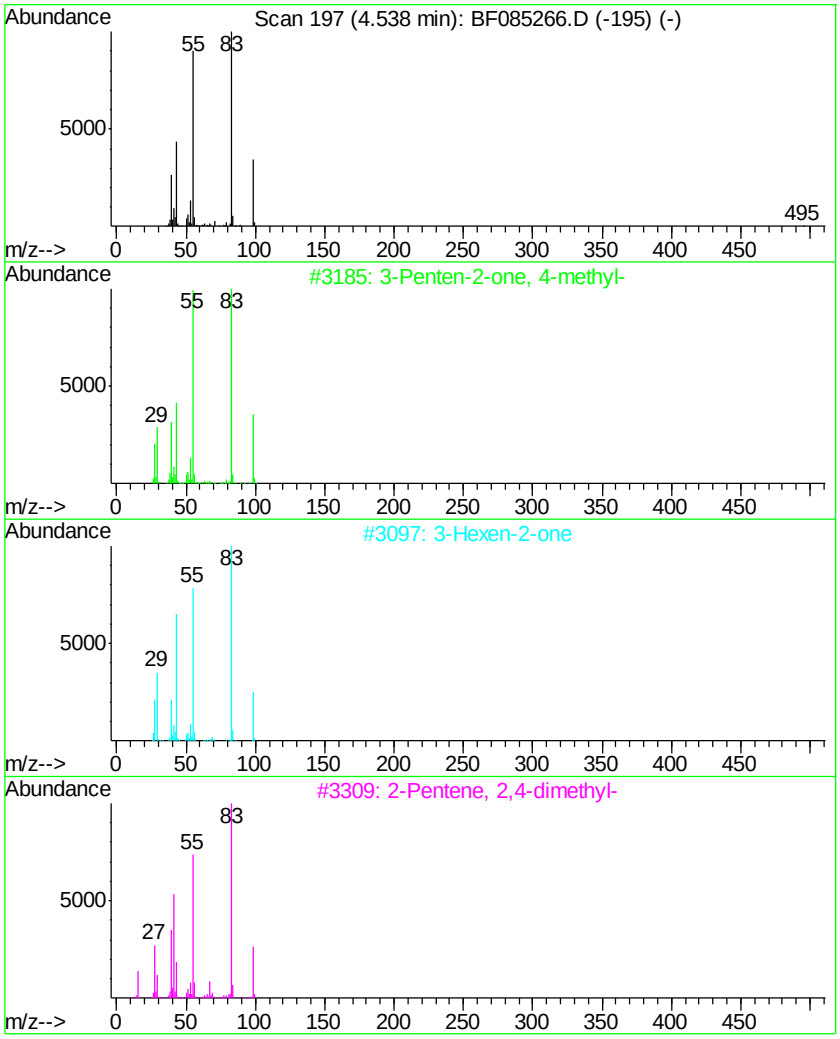
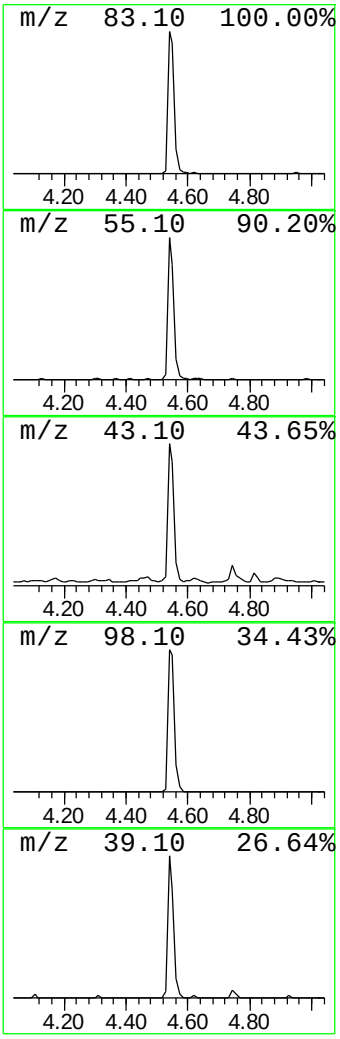
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.54	6.98 ng	309212	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085266.D
Acq On : 8 Mar 2016 20:13
Operator : UM/SJ
Sample : H1684-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RW-48-S2 GRID 3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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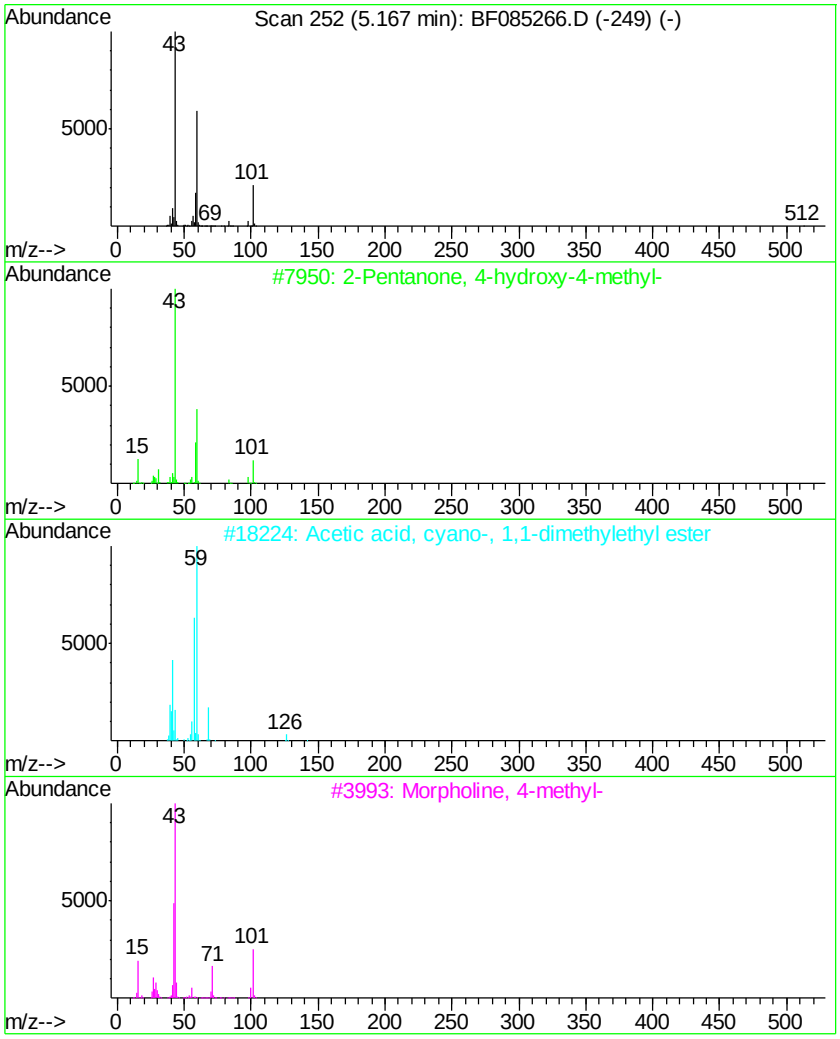
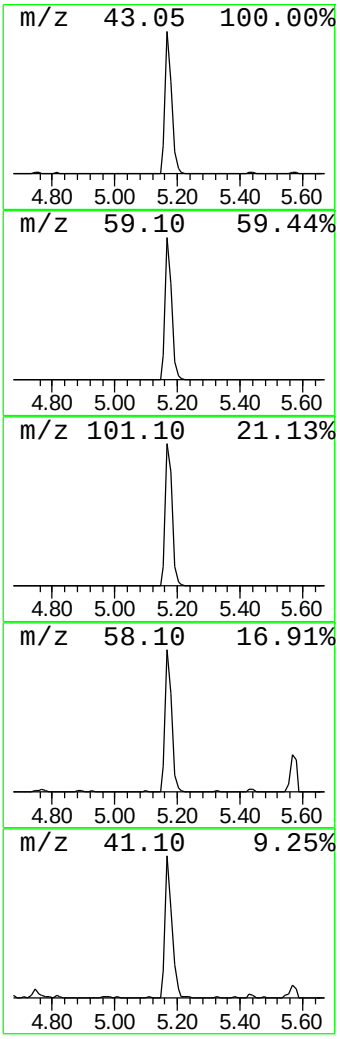
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	27.24 ng	1207620	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085266.D
Acq On : 8 Mar 2016 20:13
Operator : UM/SJ
Sample : H1684-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RW-48-S2 GRID 3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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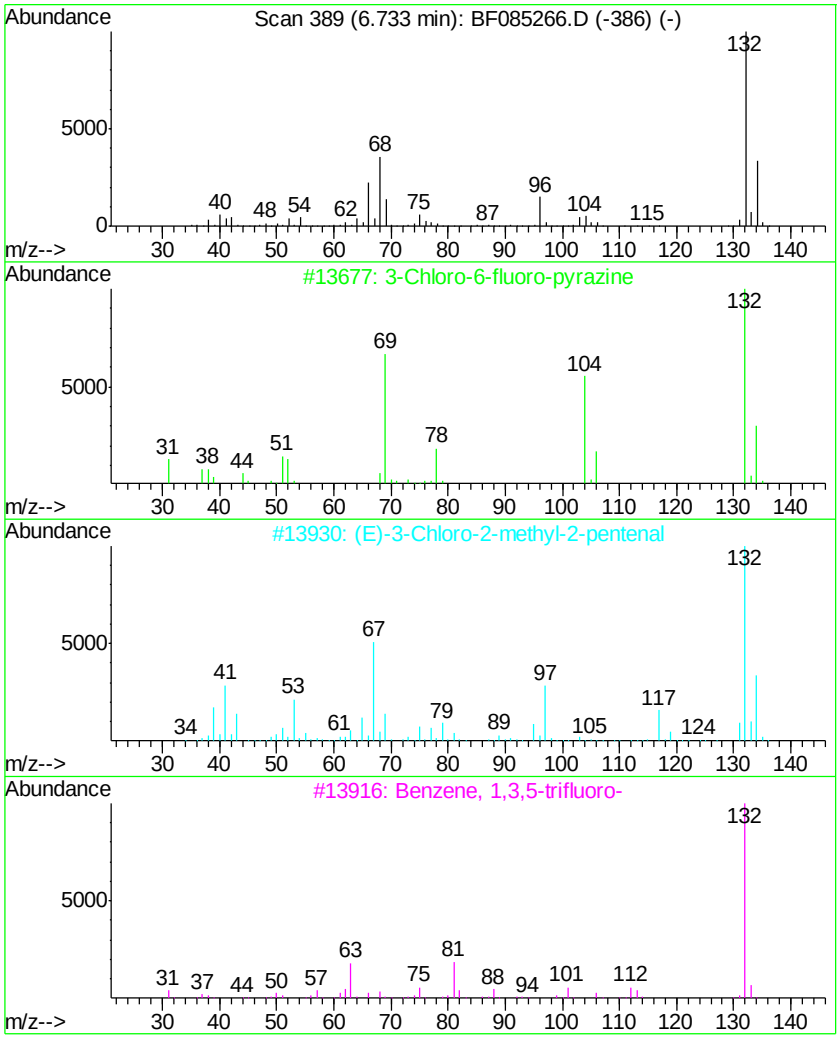
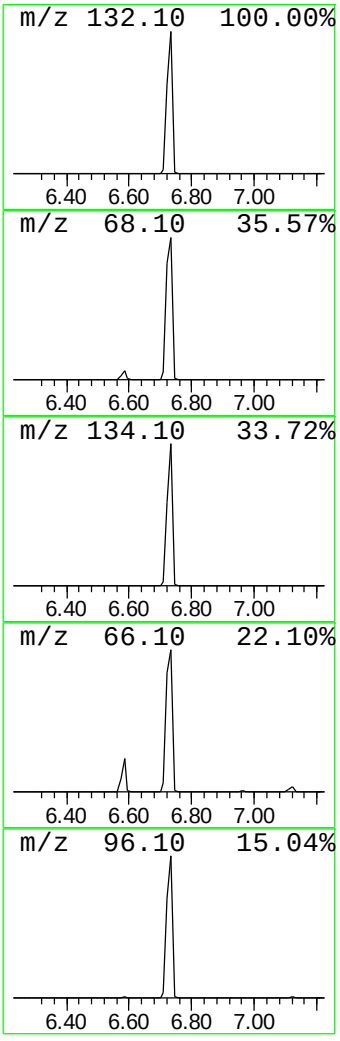
Peak Number 4 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	94.74 ng	4199980	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
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Operator : UM/SJ
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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RW-48-S2 GRID 3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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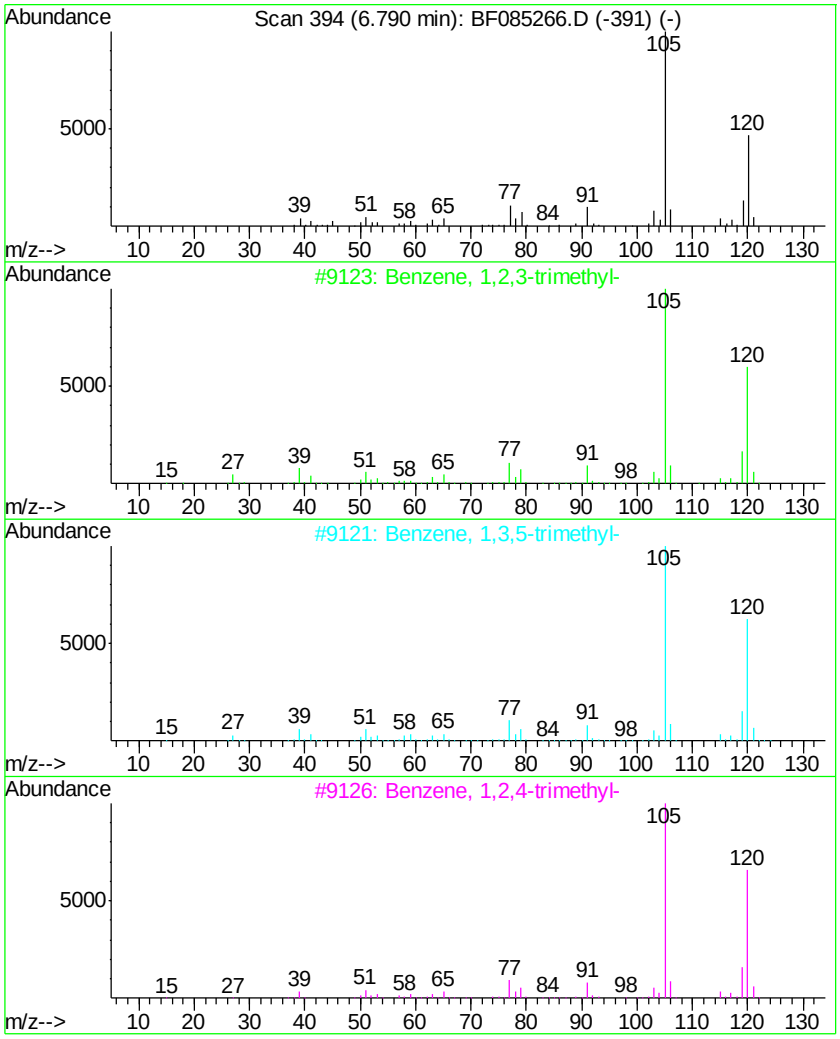
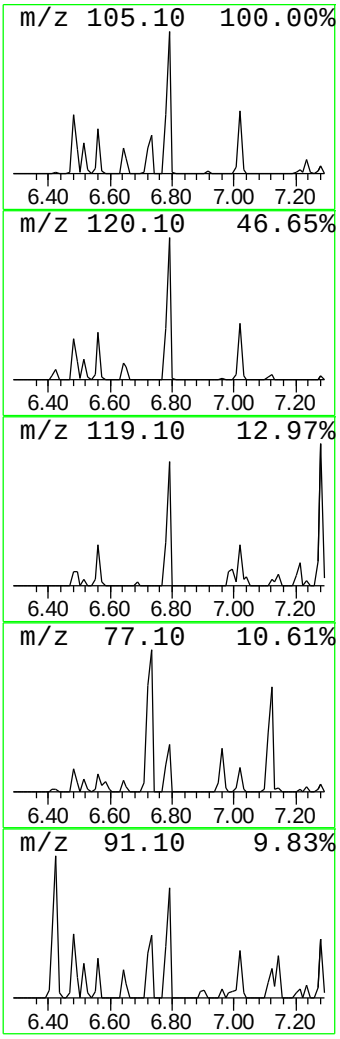
Peak Number 5 Benzene, 1,2,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.79	4.49 ng	199259	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2	Benzene, 1,3,5-trimethyl-	120	C9H12	000108-67-8	95
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	95
4	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90





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Instrument : BNA_F
ClientSampleId : RW-48-S2 GRID 3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

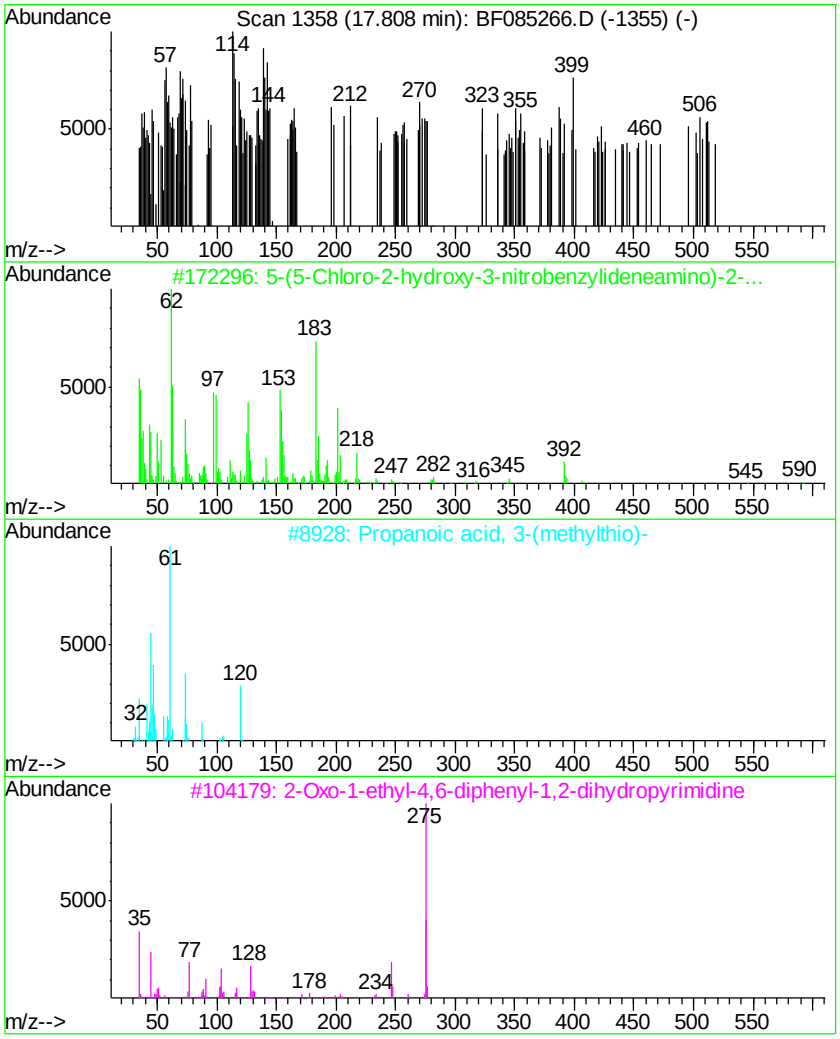
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

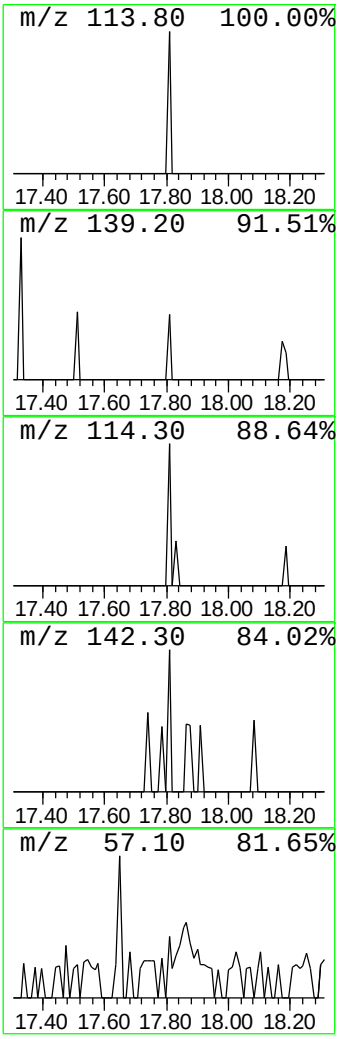
****

Peak Number 8 unknown17.81 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.81	3.65 ng	127726	Perylene-d12	15.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-(5-Chloro-2-hydroxy-3-nitroben...	590	C27H16Cl2N6O6	1000223-92-8	25
2	Propanoic acid, 3-(methylthio)-	120	C4H8O2S	000646-01-5	11
3	2-Oxo-1-ethyl-4,6-diphenyl-1,2-d...	276	C18H16N2O	033098-30-5	10
4	Butanenitrile, 4-(methylthio)-	115	C5H9NS	059121-24-3	10
5	Pyrrolidine, 1-[8-(2-octylcyclop...	349	C23H43NO	056630-59-2	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085266.D
Acq On : 8 Mar 2016 20:13
Operator : UM/SJ
Sample : H1684-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RW-48-S2 GRID 3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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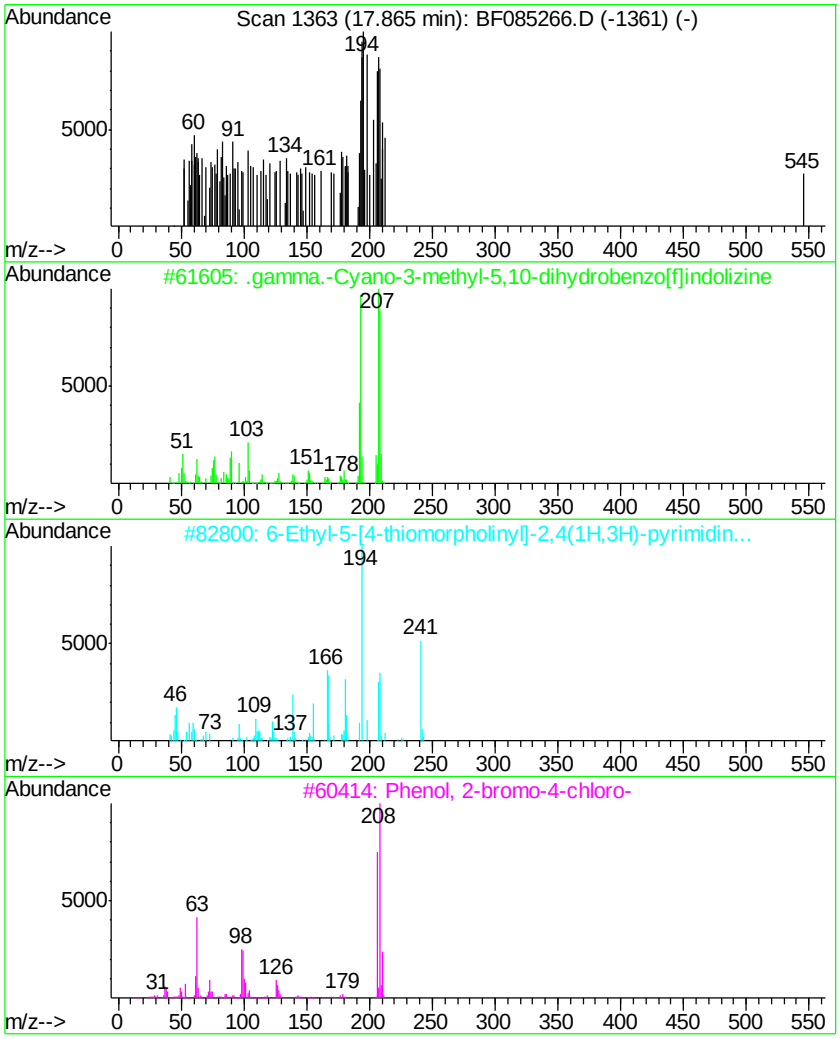
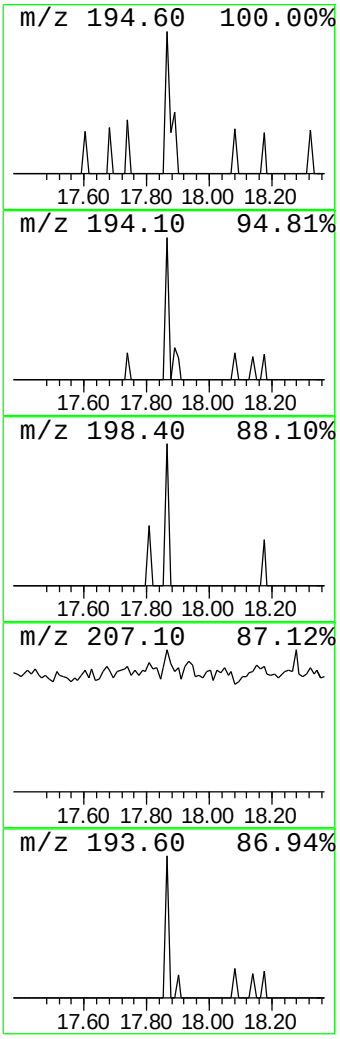
Peak Number 9 unknown17.87 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.87	2.33 ng	81642	Perylene-d12	15.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Cyano-3-methyl-5,10-dihy...	208	C14H12N2	1000213-00-8	27
2	6-Ethyl-5-[4-thiomorpholinyl]-2,...	241	C10H15N3O2S	177941-51-4	27
3	Phenol, 2-bromo-4-chloro-	206	C6H4BrClO	000695-96-5	25
4	Acetic acid, [1-methoxycarbonylb...	238	C13H18O4	1000196-65-8	14
5	7-Chloro-4-hydroxy-3-methylquino...	193	C10H8ClNO	1000213-49-2	11





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085266.D
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	2.86	3.3	ng	146177	1	6.96	886589	20.0
3-Penten-2-one, 4...	4.54	7.0	ng	309212	1	6.96	886589	20.0
2-Pentanone, 4-hy...	5.17	27.2	ng	1207620	1	6.96	886589	20.0
unknown6.73	6.73	94.7	ng	4199980	1	6.96	886589	20.0
Benzene, 1,2,3-tr...	6.79	4.5	ng	199259	1	6.96	886589	20.0
unknown17.81	17.81	3.6	ng	127726	6	15.58	699824	20.0
unknown17.87	17.87	2.3	ng	81642	6	15.58	699824	20.0