LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012015\
Data File : BF076986.D
Acq On : 21 Jan 2015 5:56
Operator : IZ / TP
Sample : G1111-01
Misc : S
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBDC1-011615

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-BF011415.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	1.361	23	24	29	rVB3	5035	9199	1.45%	0.138%
2	1.441	29	31	39	rBV	59038	100350	15.82%	1.510%
3	4.013	253	256	268	rVB	40537	102405	16.14%	1.541%
4	4.962	335	339	349	rBV	309155	581489	91.67%	8.750%
5	7.305	541	544	550	rBV	314032	589859	92.99%	8.876%
6	7.396	550	552	558	rVB	353261	634344	100.00%	9.546%
7	7.910	594	597	602	rBV	102314	162906	25.68%	2.451%
8	8.230	621	625	628	rBV	250384	396119	62.45%	5.961%
9	9.202	707	710	719	rVB	222206	343422	54.14%	5.168%
10	10.814	848	851	855	rBV	145544	223672	35.26%	3.366%
11	12.288	977	980	984	rBV2	4256	7619	1.20%	0.115%
12	13.465	1080	1083	1087	rBV	323408	518098	81.67%	7.797%
13	14.540	1174	1177	1180	rBV	23428	33211	5.24%	0.500%
14	14.951	1209	1213	1216	rBV	149174	248763	39.22%	3.743%
15	15.397	1249	1252	1260	rBV2	5359	11500	1.81%	0.173%
16	16.574	1353	1355	1357	rBV	15135	17898	2.82%	0.269%
17	16.631	1357	1360	1363	rBV	317591	408055	64.33%	6.141%
18	17.729	1454	1456	1459	rBV	194474	269169	42.43%	4.051%
19	17.900	1469	1471	1476	rVB	5220	8456	1.33%	0.127%
20	19.432	1601	1605	1607	rVB2	91619	139883	22.05%	2.105%
21	19.694	1626	1628	1630	rBV	13693	15621	2.46%	0.235%
22	19.969	1649	1652	1654	rVB	392613	503545	79.38%	7.578%
23	20.346	1679	1685	1687	rBV3	3139	7205	1.14%	0.108%
24	20.940	1734	1737	1740	rBV3	2183	6355	1.00%	0.096%
25	21.237	1758	1763	1765	rBV	214429	345265	54.43%	5.196%
26	21.363	1772	1774	1776	rBV2	12335	15833	2.50%	0.238%
27	21.626	1794	1797	1799	rBV3	5689	9895	1.56%	0.149%
28	21.935	1821	1824	1825	rVB3	7605	10176	1.60%	0.153%
29	22.015	1828	1831	1833	rBV	27782	40061	6.32%	0.603%
30	22.392	1861	1864	1867	rVB4	8766	16437	2.59%	0.247%
31	22.449	1867	1869	1870	rBV2	10012	12636	1.99%	0.190%
32	22.483	1870	1872	1874	rVV2	9760	14589	2.30%	0.220%
33	22.758	1893	1896	1901	rBV2	95259	141544	22.31%	2.130%
34	22.838	1901	1903	1905	rVV	9723	15017	2.37%	0.226%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012015\
Data File : BF076986.D
Acq On : 21 Jan 2015 5:56
Operator : IZ / TP
Sample : G1111-01
Misc : S
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBDC1-011615

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-BF011415.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	22.895	1905	1908	1912	rVV	208955	263713	41.57%	3.968%
36	22.963	1912	1914	1916	rVV3	4567	7979	1.26%	0.120%
37	23.123	1926	1928	1931	rBV2	5219	11176	1.76%	0.168%
38	23.295	1941	1943	1946	rVB4	13586	18347	2.89%	0.276%
39	23.500	1958	1961	1967	rBV4	21656	64515	10.17%	0.971%
40	23.581	1967	1968	1972	rVB3	7939	11907	1.88%	0.179%
41	23.821	1987	1989	1990	rBV2	5864	6368	1.00%	0.096%
42	24.061	2005	2010	2012	rBV2	19089	45338	7.15%	0.682%
43	24.152	2016	2018	2020	rBV3	6073	12160	1.92%	0.183%
44	24.255	2025	2027	2030	rBV4	7101	11191	1.76%	0.168%
45	24.323	2030	2033	2036	rVV4	13005	25068	3.95%	0.377%
46	24.472	2044	2046	2050	rBV5	18472	39328	6.20%	0.592%
47	24.563	2050	2054	2058	rBV7	11672	37162	5.86%	0.559%
48	24.735	2066	2069	2072	rBV4	9658	19865	3.13%	0.299%
49	24.964	2086	2089	2095	rBV7	12555	44005	6.94%	0.662%
50	25.501	2134	2136	2137	rBV2	4522	8749	1.38%	0.132%
51	25.649	2148	2149	2154	rBV5	4587	12254	1.93%	0.184%
52	25.764	2157	2159	2166	rVB8	12746	37027	5.84%	0.557%
53	25.889	2168	2170	2173	rBV3	4647	8490	1.34%	0.128%

Sum of corrected areas: 6645238

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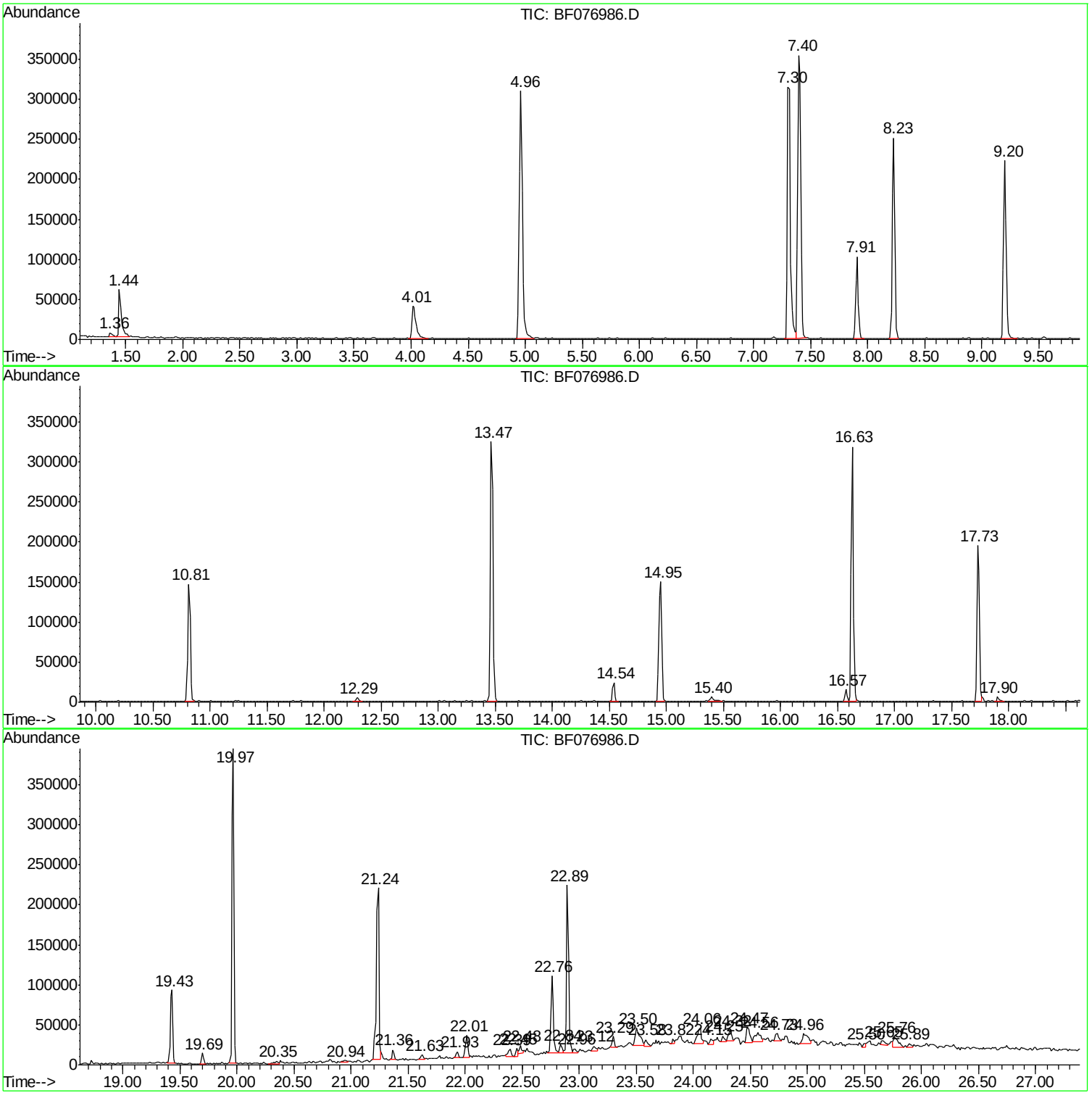
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBDC1-011615

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.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

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012015\
Data File : BF076986.D
Acq On : 21 Jan 2015 5:56
Operator : IZ / TP
Sample : G1111-01
Misc : S
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBDC1-011615

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.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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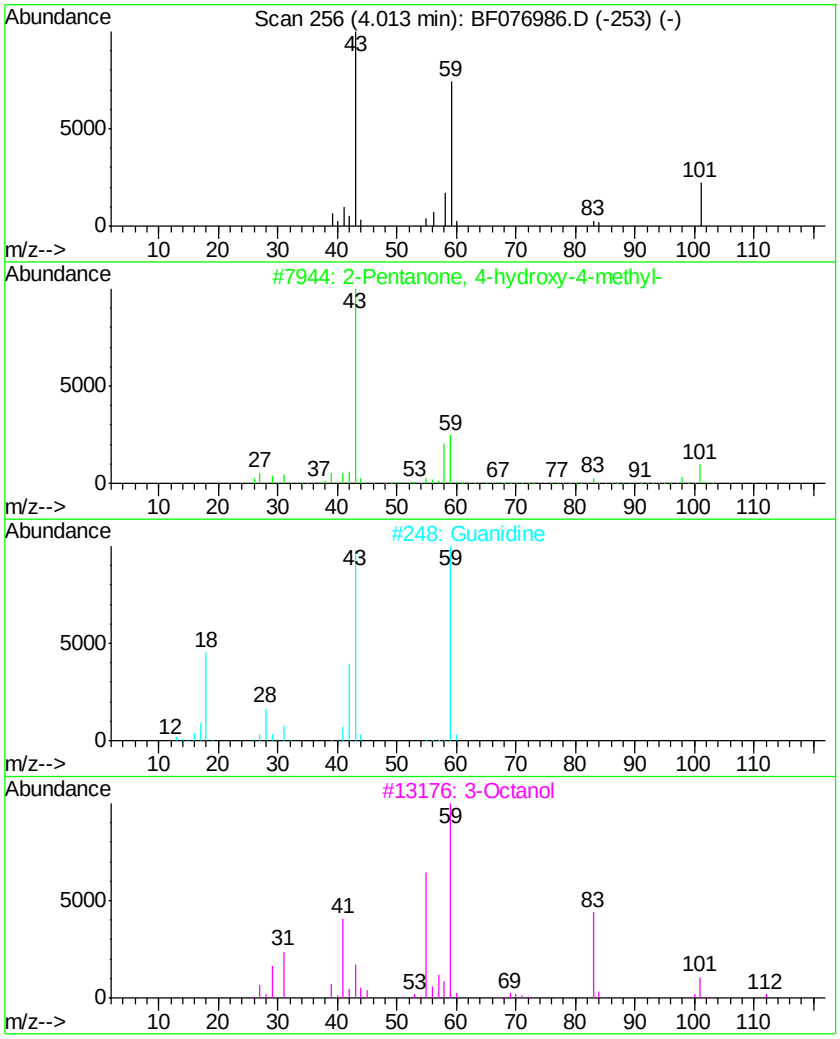
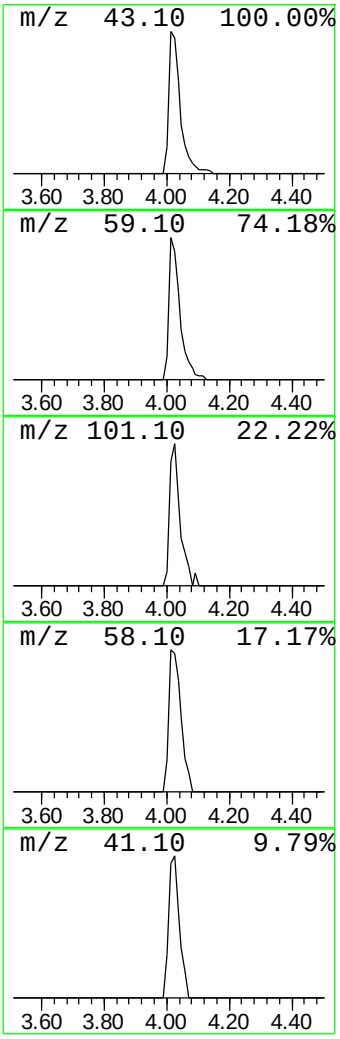
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.01	12.57 ng	102405	1,4-Dichlorobenzene-d4	7.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Guanidine	59	CH5N3	000113-00-8	53
3	3-Octanol	130	C8H18O	000589-98-0	36
4	Acetone	58	C3H6O	000067-64-1	9
5	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012015\
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Operator : IZ / TP
Sample : G1111-01
Misc : S
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBDC1-011615

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.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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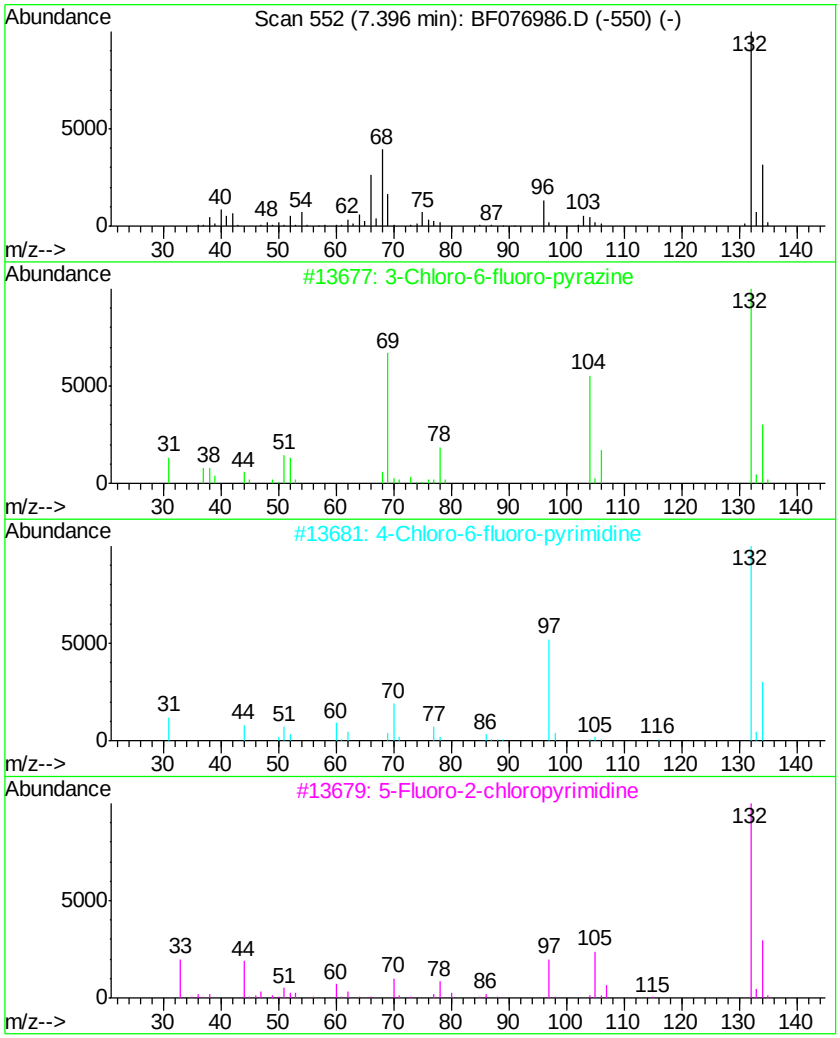
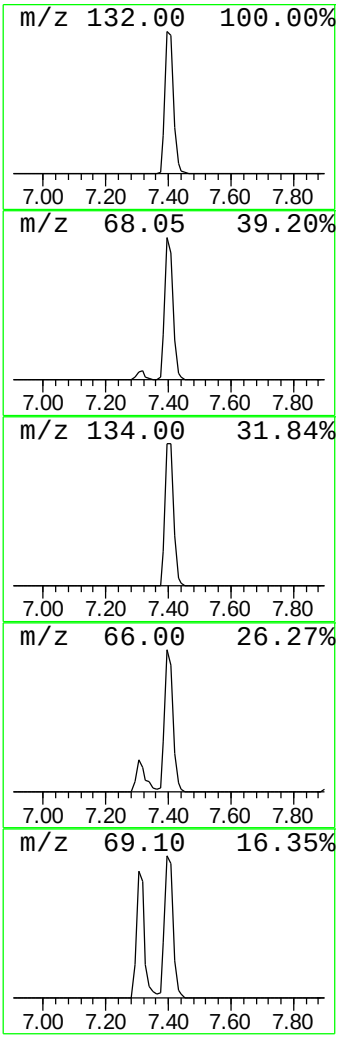
Peak Number 3 unknown7.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.40	77.88 ng	634344	1,4-Dichlorobenzene-d4	7.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012015\
Data File : BF076986.D
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Operator : IZ / TP
Sample : G1111-01
Misc : S
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBDC1-011615

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.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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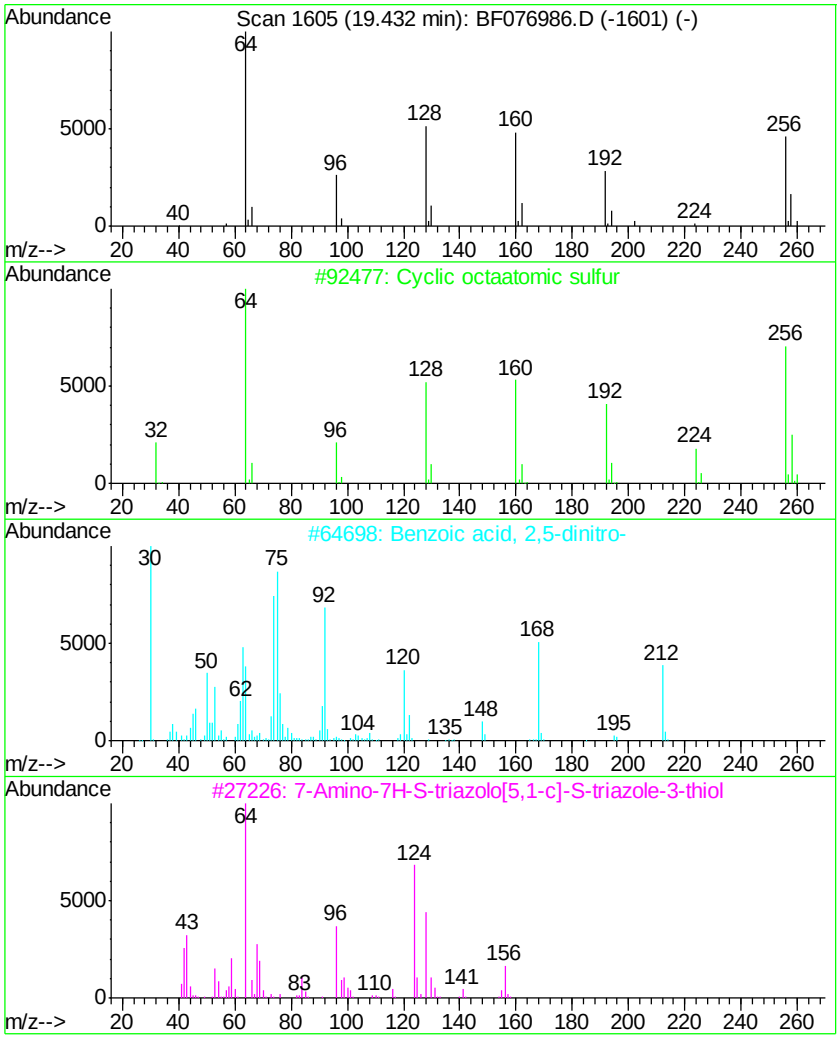
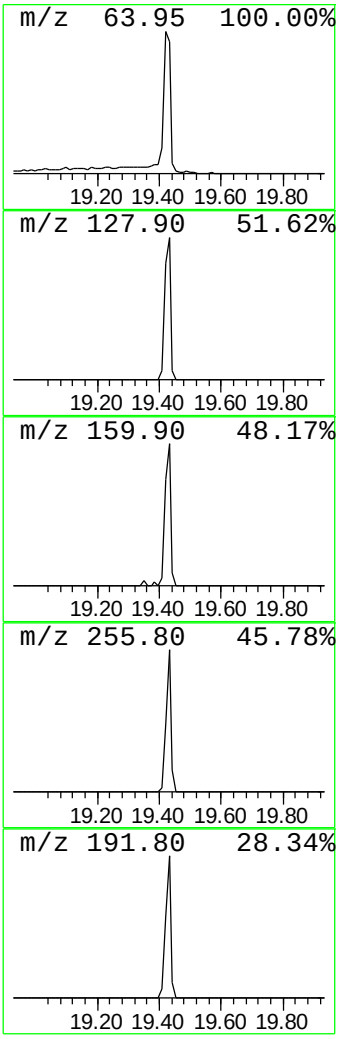
Peak Number 5 Cyclic octaatomic sulfur Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.43	10.39 ng	139883	Phenanthrene-d10	17.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclic octaatomic sulfur	256	S8	010544-50-0	97
2	Benzoic acid, 2,5-dinitro-	212	C7H4N2O6	000610-28-6	47
3	7-Amino-7H-S-triazolo[5,1-c]-S-t...	156	C3H4N6S	013728-28-4	36
4	1,2,5,6-Tetrathiocane	184	C4H8S4	001940-01-8	9
5	2,3-Diazabicyclo[3.2.0]hept-2-en...	176	C7H7F3N2	1000258-92-2	9





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ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBDC1-011615

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.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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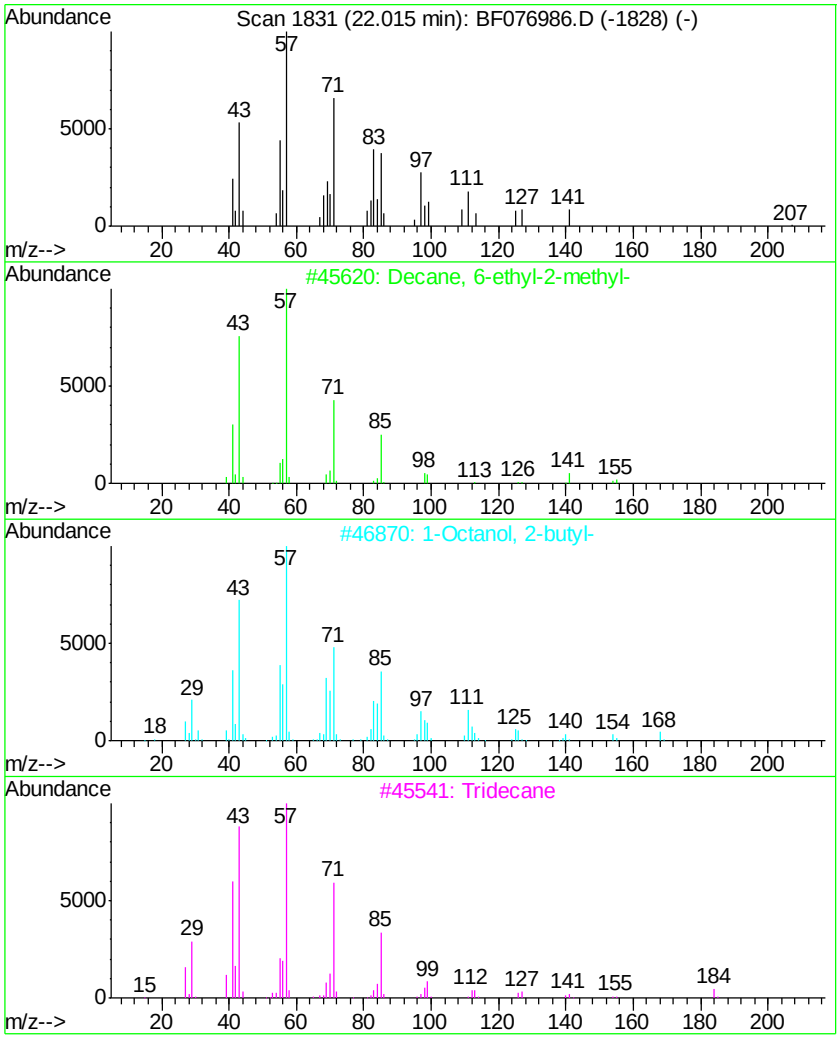
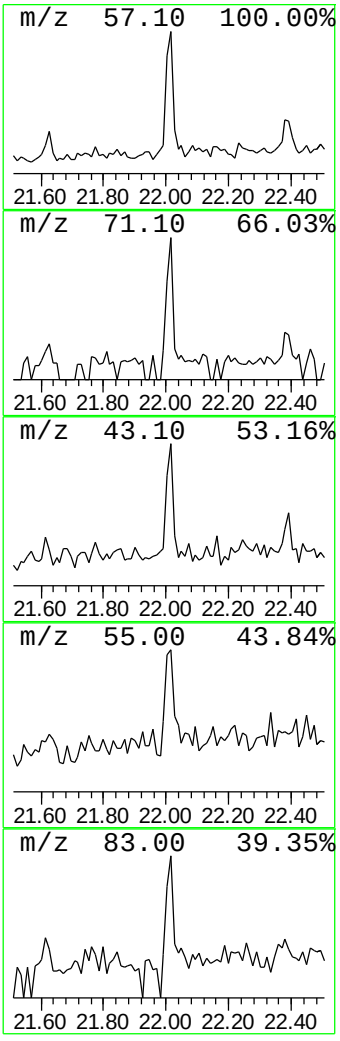
Peak Number 6 unknown22.01 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.01	2.32 ng	40061	Chrysene-d12	21.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	47
2	1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	47
3	Tridecane	184	C13H28	000629-50-5	47
4	Octacosane	394	C28H58	000630-02-4	47
5	Nonacosane	408	C29H60	000630-03-5	47





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Misc : S
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBDC1-011615

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.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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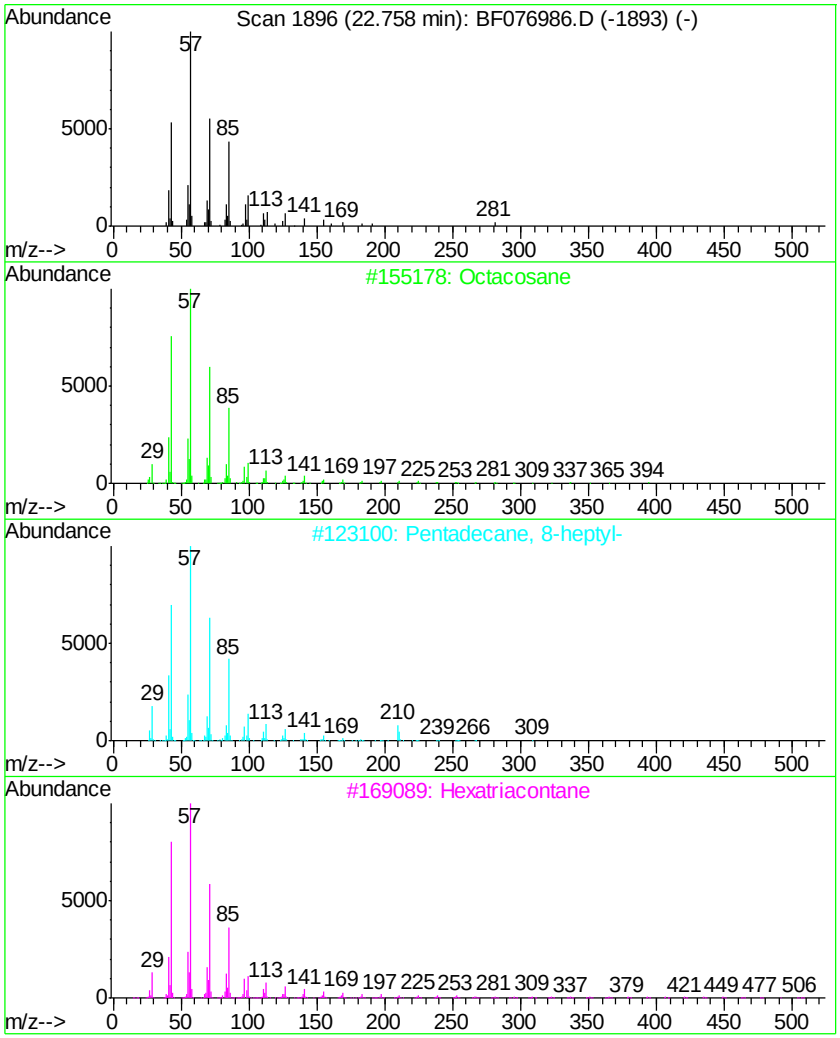
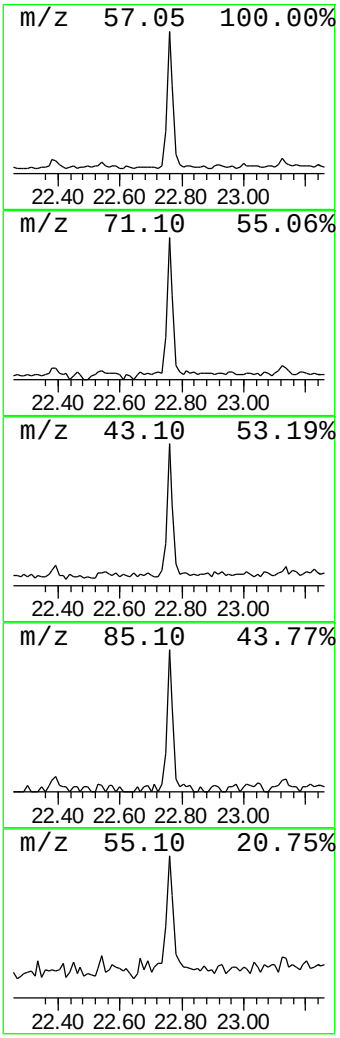
Peak Number 7 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.76	10.73 ng	141544	Perylene-d12	22.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
3	Hexatriacontane	507	C36H74	000630-06-8	91
4	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	90
5	Heneicosane	296	C21H44	000629-94-7	87





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ClientSampleId : RBDC1-011615

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.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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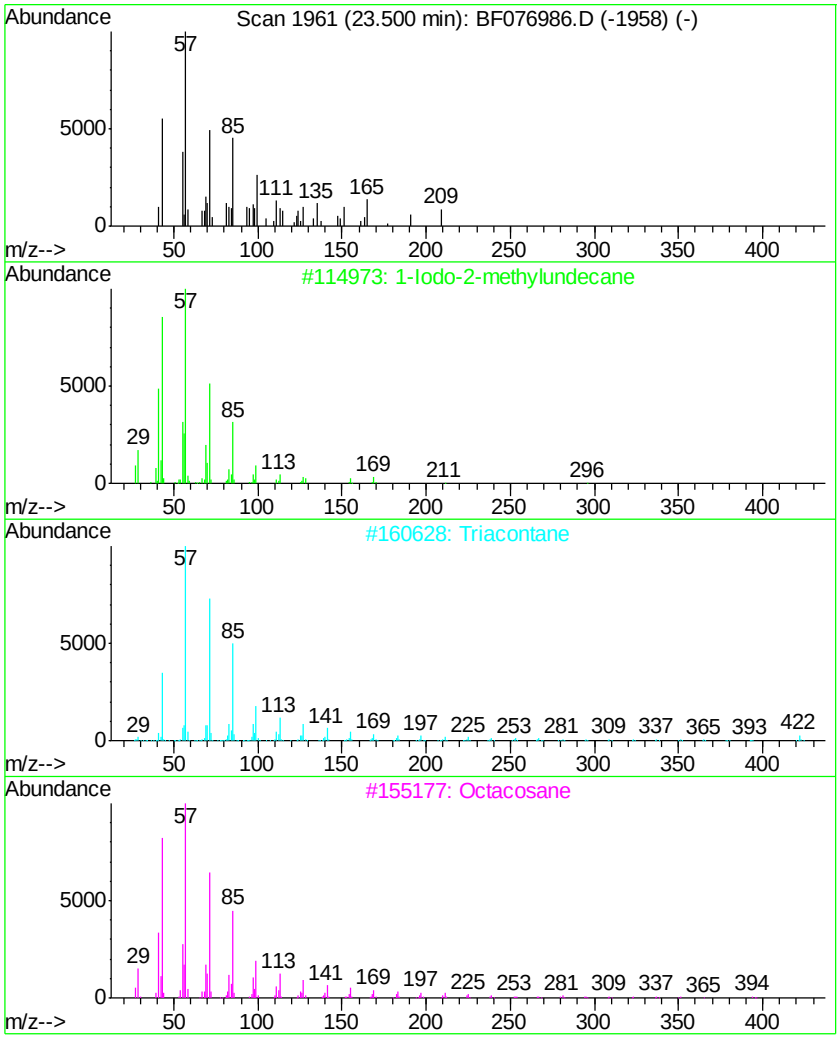
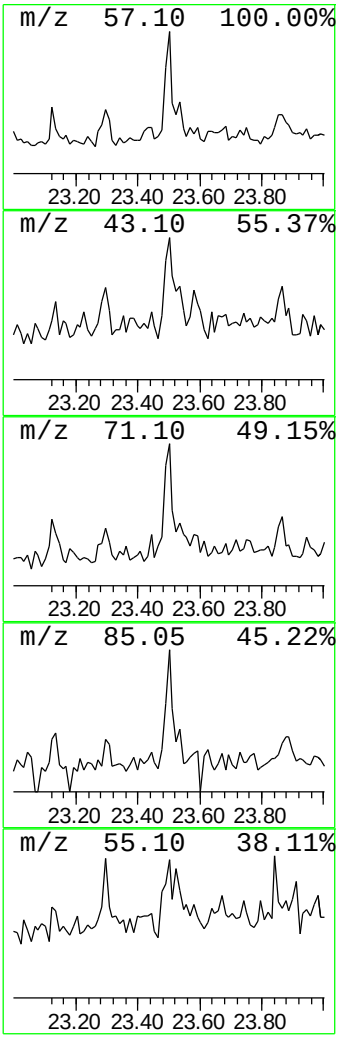
Peak Number 8 1-Iodo-2-methylundecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.50	4.89 ng	64515	Perylene-d12	22.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	53
2	Triacontane	422	C30H62	000638-68-6	53
3	Octacosane	394	C28H58	000630-02-4	53
4	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	50
5	Undecane	156	C11H24	001120-21-4	43





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Instrument : BNA_F
ClientSampleId : RBDC1-011615

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.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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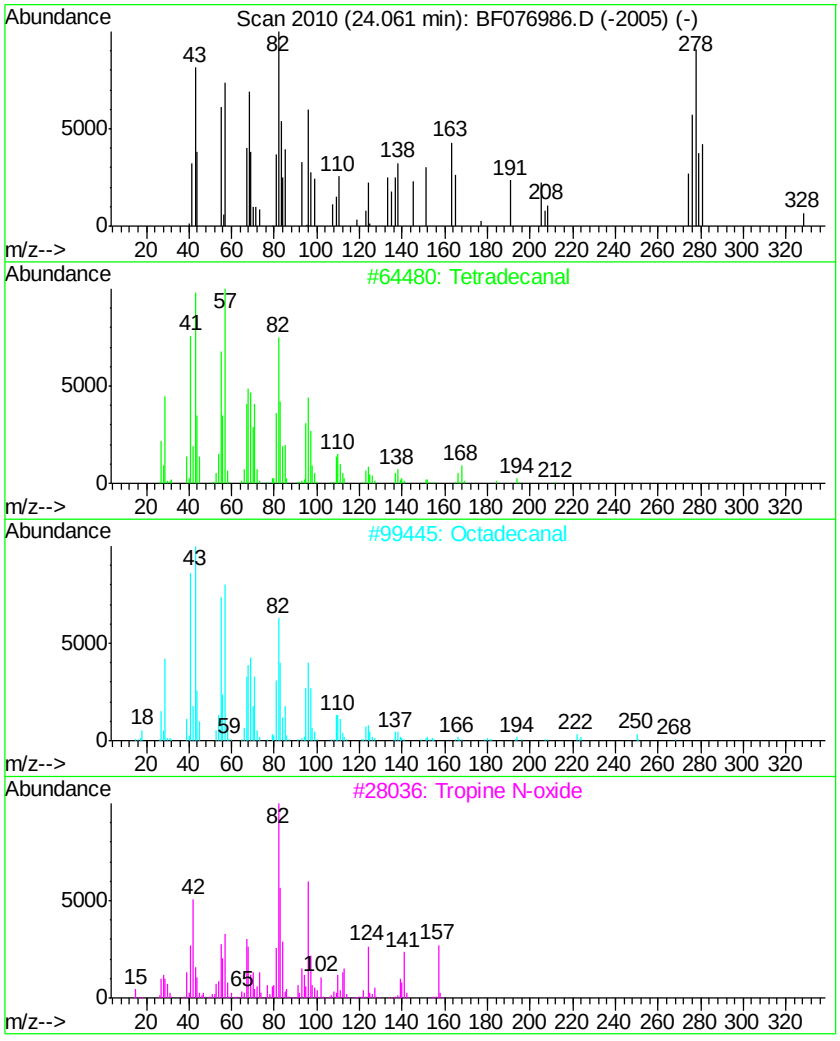
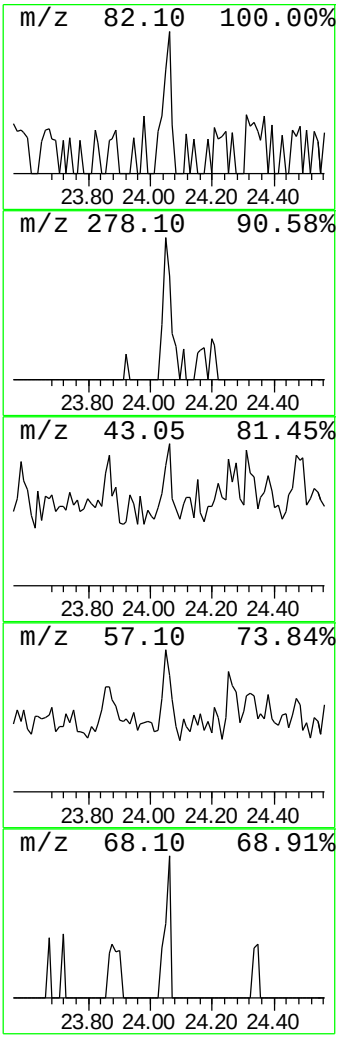
Peak Number 9 unknown24.06 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.06	3.44 ng	45338	Perylene-d12	22.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanal	212	C14H28O	000124-25-4	22
2	Octadecanal	268	C18H36O	000638-66-4	22
3	Tropine N-oxide	157	C8H15NO2	035722-43-1	14
4	8-Azabicyclo[3.2.1]octan-3-ol, 8...	157	C8H15NO2	032663-71-1	14
5	Z-2-Octadecen-1-ol	268	C18H36O	1000131-11-0	14





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012015\
Data File : BF076986.D
Acq On : 21 Jan 2015 5:56
Operator : IZ / TP
Sample : G1111-01
Misc : S
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBDC1-011615

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.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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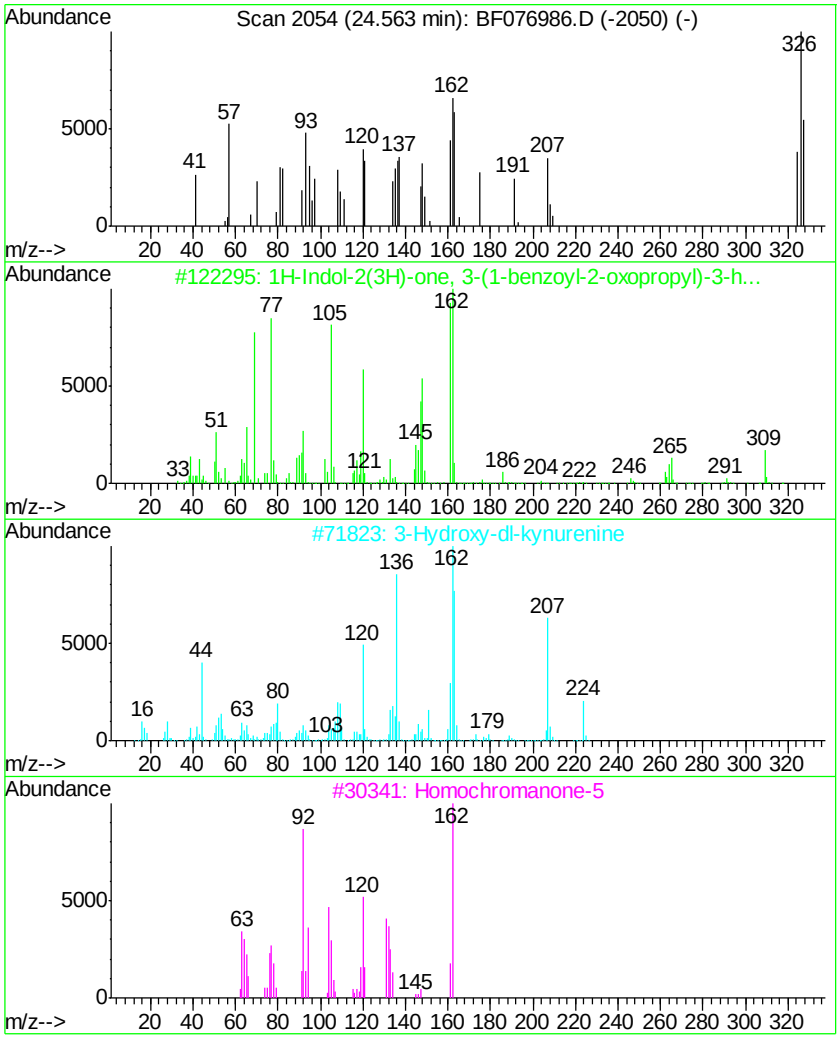
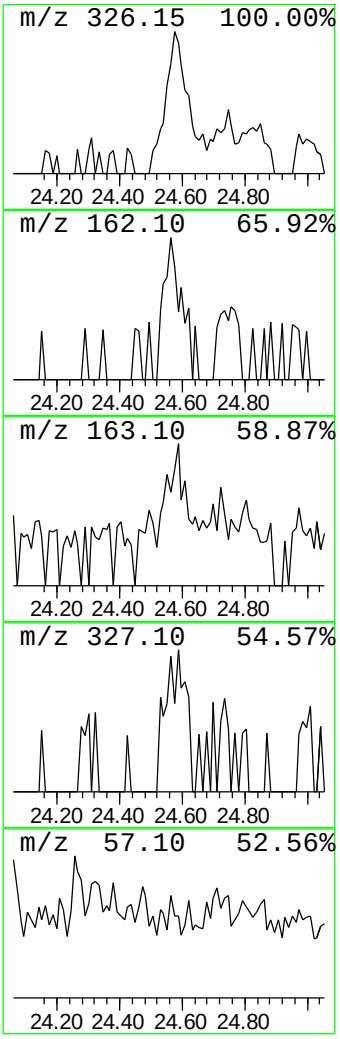
Peak Number 11 unknown24.56 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.56	2.82 ng	37162	Perylene-d12	22.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indol-2(3H)-one, 3-(1-benzoyl...	309	C18H15NO4	076325-78-5	22
2	3-Hydroxy-dl-kynurenine	224	C10H12N2O4	002147-61-7	17
3	Homochromanone-5	162	C10H10O2	006786-30-7	11
4	Methanimidamide, N-(2,4-dimethyl...	162	C10H14N2	033089-74-6	10
5	Disiloxane, 1,3-diethoxy-1,1,3,3...	222	C8H22O3Si2	018420-09-2	10





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012015\
Data File : BF076986.D
Acq On : 21 Jan 2015 5:56
Operator : IZ / TP
Sample : G1111-01
Misc : S
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBDC1-011615

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

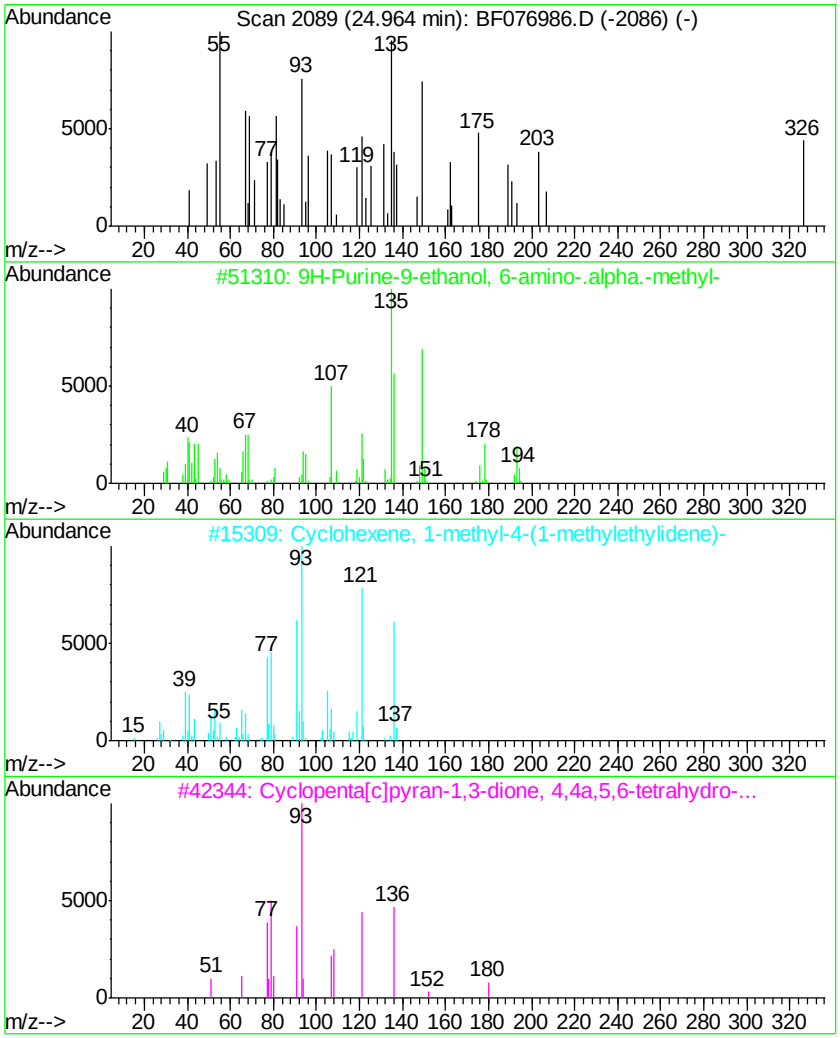
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

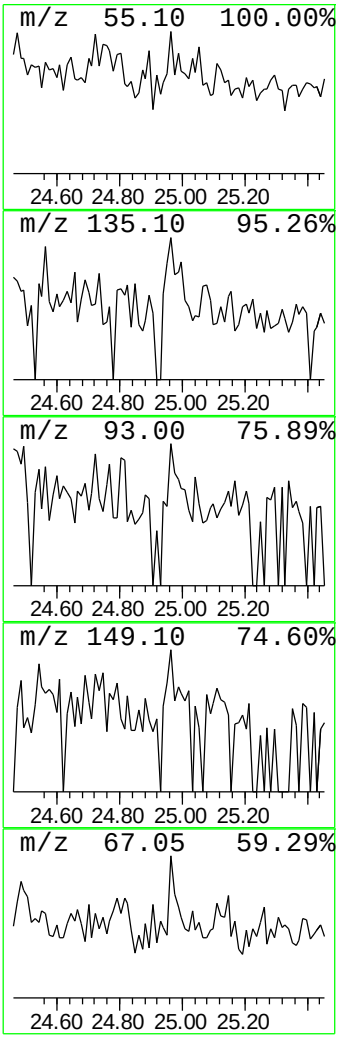
****

Peak Number 12 unknown24.96 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.96	3.34 ng	44005	Perylene-d12	22.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9H-Purine-9-ethanol, 6-amino-.al...	193	C8H11N5O	000712-00-5	14
2	Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	000586-62-9	11
3	Cyclopenta[c]pyran-1,3-dione, 4,...	180	C10H12O3	066407-26-9	10
4	Cyclopentene, 3-isopropenyl-5,5-...	136	C10H16	1000162-25-4	10
5	(+)-4-Carene	136	C10H16	029050-33-7	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012015\
Data File : BF076986.D
Acq On : 21 Jan 2015 5:56
Operator : IZ / TP
Sample : G1111-01
Misc : S
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBDC1-011615

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.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
2-Pentanone, 4-hy...	4.01	12.6	ng	102405	1	7.91	162906	20.0
unknown7.40	7.40	77.9	ng	634344	1	7.91	162906	20.0
Cyclic octaatomic...	19.43	10.4	ng	139883	4	17.73	269169	20.0
unknown22.01	22.01	2.3	ng	40061	5	21.24	345265	20.0
Octacosane	22.76	10.7	ng	141544	6	22.89	263713	20.0
1-Iodo-2-methylun...	23.50	4.9	ng	64515	6	22.89	263713	20.0
unknown24.06	24.06	3.4	ng	45338	6	22.89	263713	20.0
unknown24.56	24.56	2.8	ng	37162	6	22.89	263713	20.0
unknown24.96	24.96	3.3	ng	44005	6	22.89	263713	20.0