LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091115\
Data File : BF081596.D
Acq On : 11 Sep 2015 22:24
Operator : UM/IZ
Sample : G3558-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

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-BF090115.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	1.463	10	11	17	rBV	27417	62951	3.70%	0.420%
2	1.554	17	19	44	rVB	180063	562631	33.04%	3.753%
3	2.605	107	111	114	rVB	18065	30309	1.78%	0.202%
4	4.560	277	282	298	rBV	349043	974693	57.23%	6.502%
5	5.417	354	357	374	rVB	820121	1645316	96.61%	10.976%
6	7.680	551	555	559	rBV	921244	1703085	100.00%	11.361%
7	7.772	559	563	566	rVB	991067	1649137	96.83%	11.001%
8	8.252	601	605	610	rBB	205600	339388	19.93%	2.264%
9	8.572	629	633	637	rBV	583753	990885	58.18%	6.610%
10	9.543	714	718	721	rBV	525340	1083902	63.64%	7.230%
11	11.143	854	858	862	rBV	261197	437659	25.70%	2.920%
12	13.795	1085	1090	1093	rBV	852198	1393352	81.81%	9.295%
13	14.847	1178	1182	1185	rBV	116589	177526	10.42%	1.184%
14	15.281	1216	1220	1224	rBB	263332	431228	25.32%	2.877%
15	17.190	1382	1387	1390	rBV	516992	979708	57.53%	6.535%
16	17.818	1440	1442	1448	rBB	7782	17817	1.05%	0.119%
17	18.790	1523	1527	1530	rBV	239949	409039	24.02%	2.729%
18	20.527	1676	1679	1687	rBV	26369	52988	3.11%	0.353%
19	21.419	1753	1757	1762	rVB2	66004	121784	7.15%	0.812%
20	21.796	1788	1790	1793	rBV	24501	30114	1.77%	0.201%
21	21.922	1799	1801	1807	rBV	12937	21570	1.27%	0.144%
22	22.047	1809	1812	1816	rVB	28131	28276	1.66%	0.189%
23	22.127	1816	1819	1821	rBV	880778	991125	58.20%	6.612%
24	22.950	1889	1891	1894	rVB	25001	24310	1.43%	0.162%
25	23.396	1925	1930	1935	rBV	290307	358369	21.04%	2.391%
26	23.533	1937	1942	1943	rBV2	10463	32438	1.90%	0.216%
27	23.728	1957	1959	1965	rVB3	20035	35901	2.11%	0.239%
28	24.059	1986	1988	1990	rBV2	15737	22810	1.34%	0.152%
29	24.493	2024	2026	2030	rBV	19967	35792	2.10%	0.239%
30	24.653	2038	2040	2044	rBV3	12555	31642	1.86%	0.211%
31	24.836	2053	2056	2058	rBV	192540	261065	15.33%	1.742%
32	27.659	2299	2303	2309	rVB5	15302	53961	3.17%	0.360%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091115\
Data File : BF081596.D
Acq On : 11 Sep 2015 22:24
Operator : UM/IZ
Sample : G3558-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2

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-BF090115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 14990771

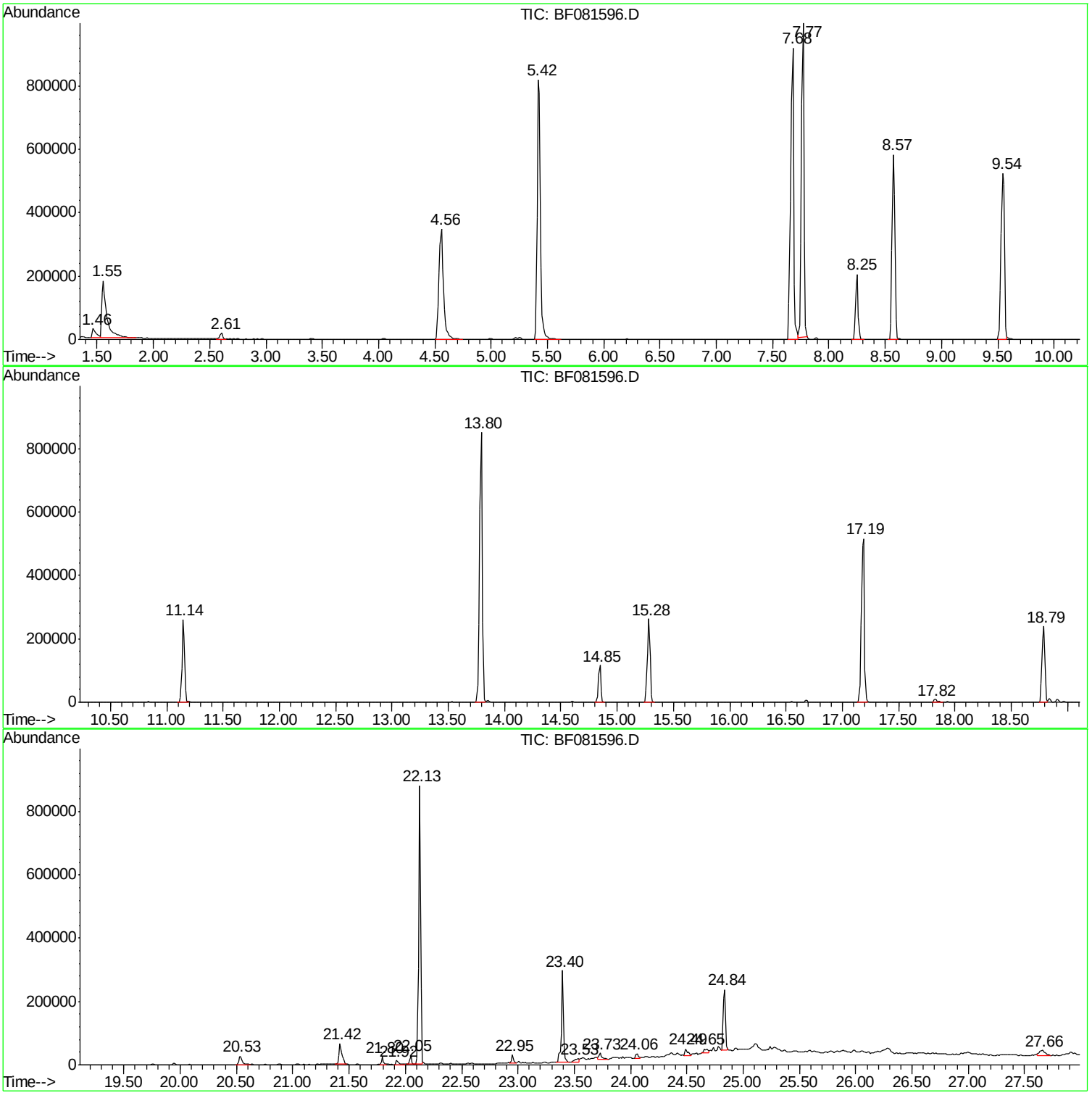
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091115\
Data File : BF081596.D
Acq On : 11 Sep 2015 22:24
Operator : UM/IZ
Sample : G3558-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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\BF091115\
Data File : BF081596.D
Acq On : 11 Sep 2015 22:24
Operator : UM/IZ
Sample : G3558-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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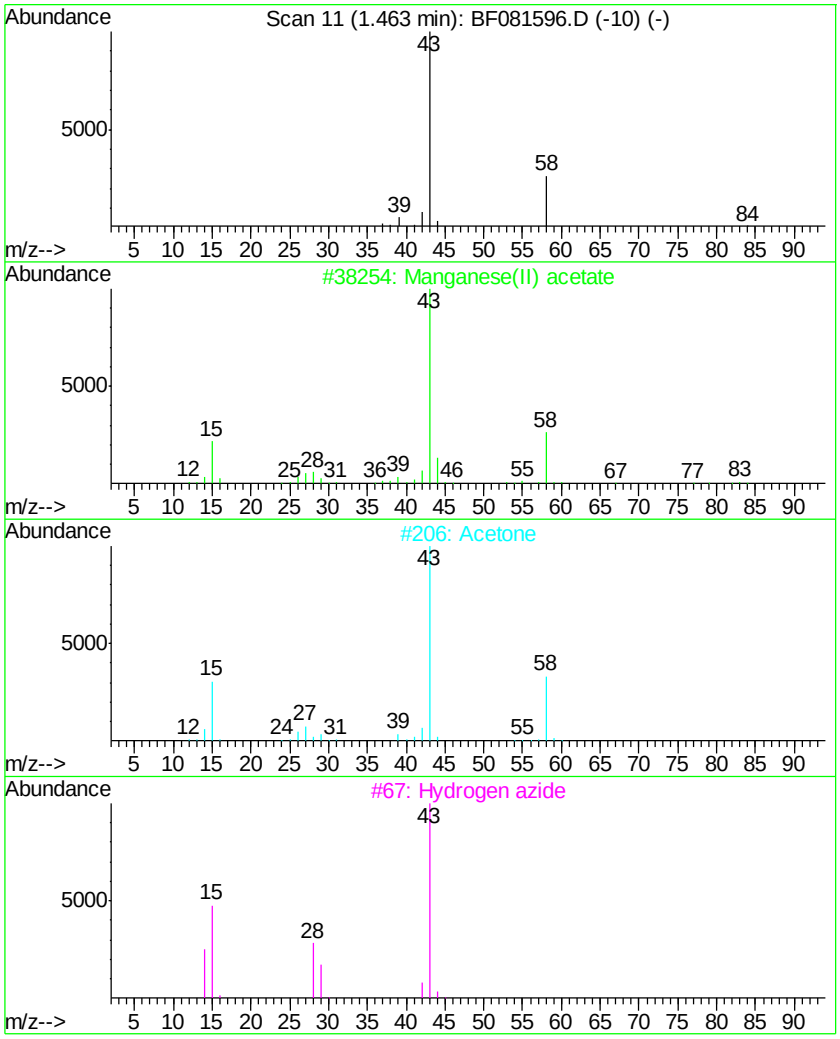
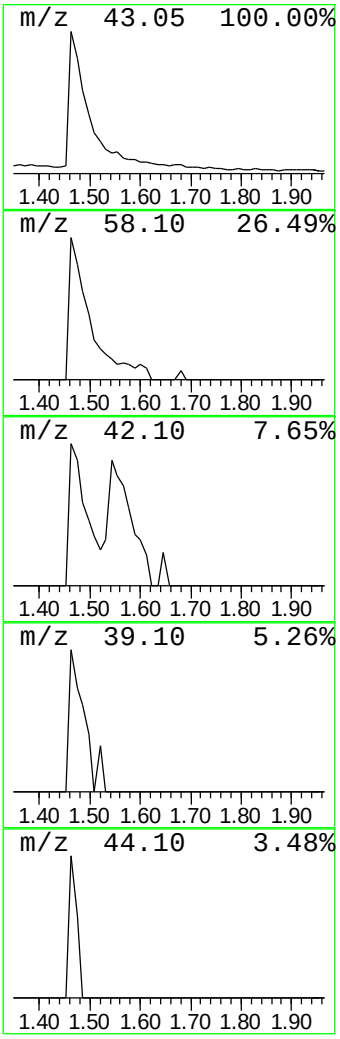
Peak Number 1 Manganese(II) acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.46	3.71 ng	62951	1,4-Dichlorobenzene-d4	8.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Manganese(II) acetate	173	C4H6MnO4	006156-78-1	56
2	Acetone	58	C3H6O	000067-64-1	9
3	Hydrogen azide	43	HN3	007782-79-8	4
4	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	4
5	Ethene, methoxy-	58	C3H6O	000107-25-5	3





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091115\
Data File : BF081596.D
Acq On : 11 Sep 2015 22:24
Operator : UM/IZ
Sample : G3558-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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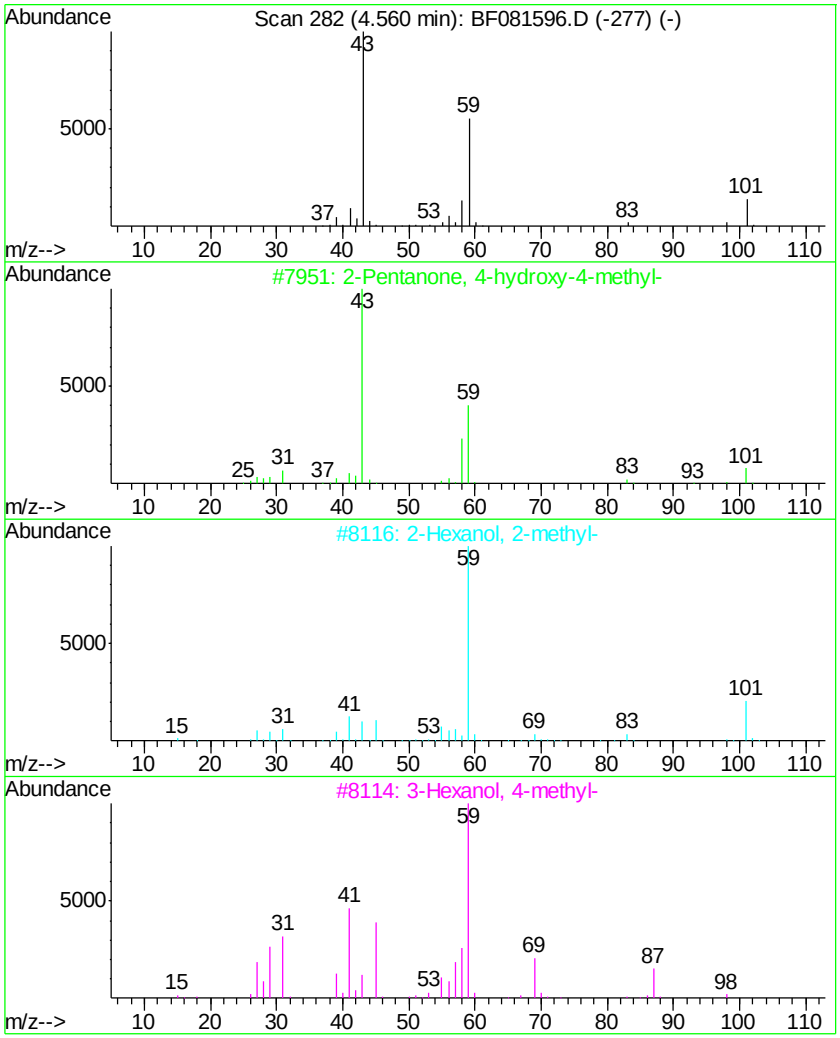
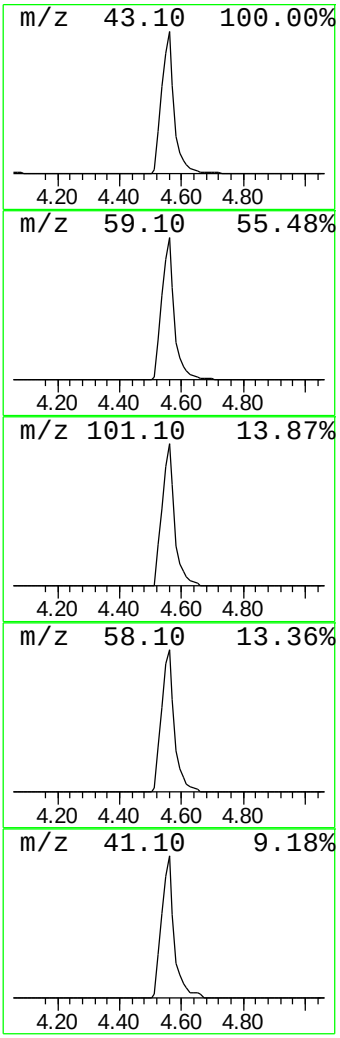
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.56	57.44 ng	974693	1,4-Dichlorobenzene-d4	8.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091115\
Data File : BF081596.D
Acq On : 11 Sep 2015 22:24
Operator : UM/IZ
Sample : G3558-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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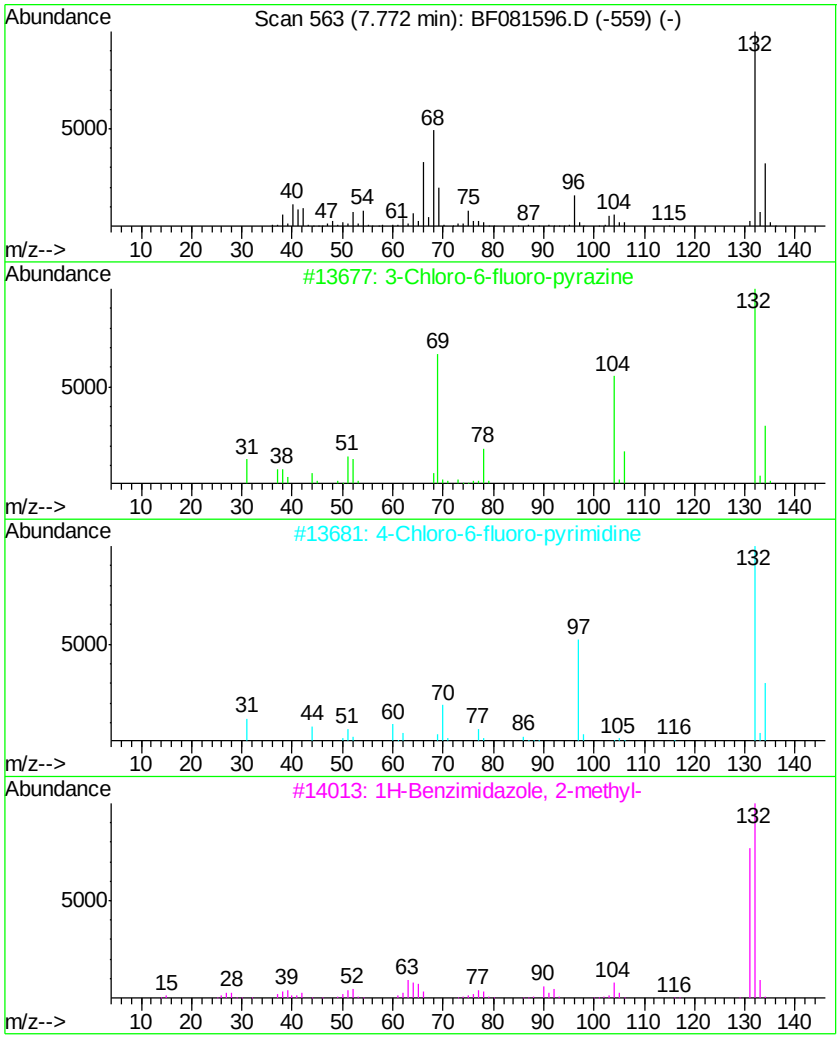
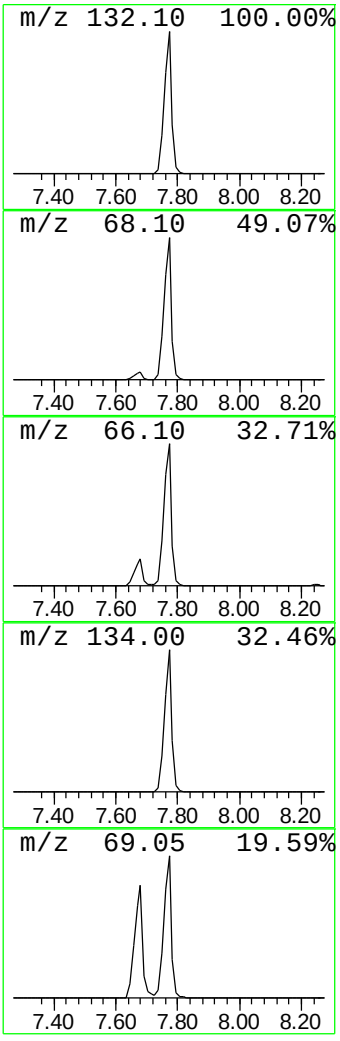
Peak Number 4 unknown7.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.77	97.18 ng	1649140	1,4-Dichlorobenzene-d4	8.25

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	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	25
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





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Data File : BF081596.D
Acq On : 11 Sep 2015 22:24
Operator : UM/IZ
Sample : G3558-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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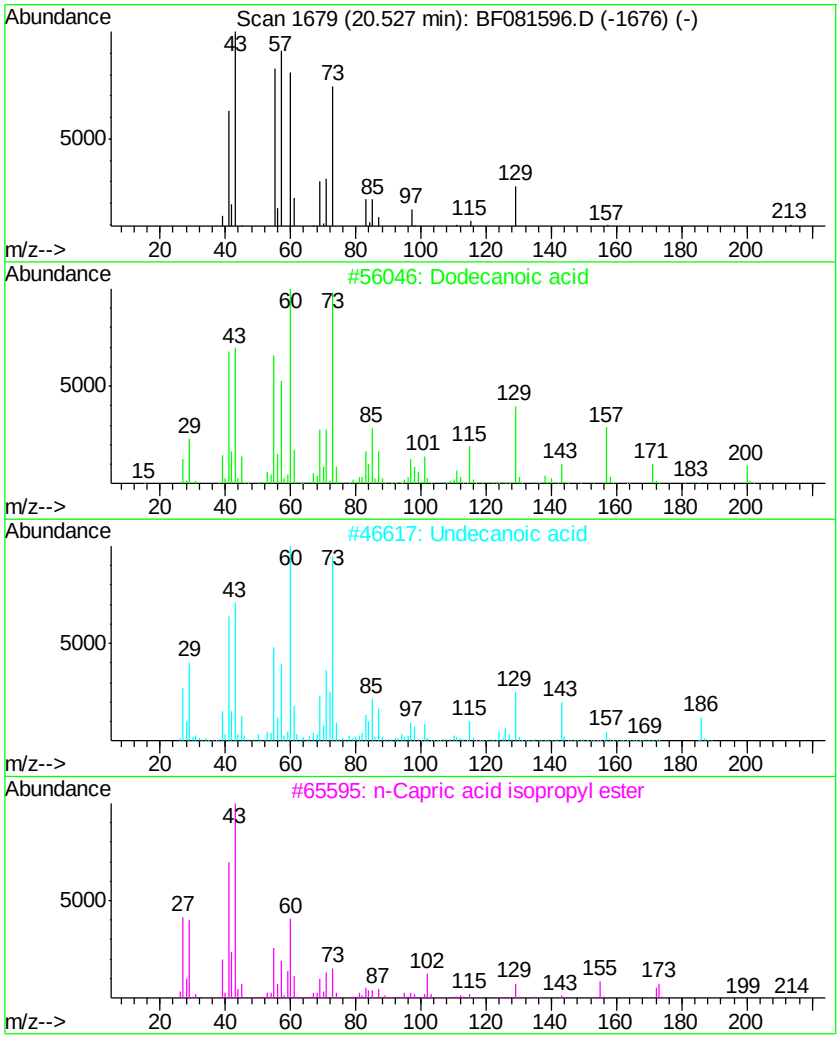
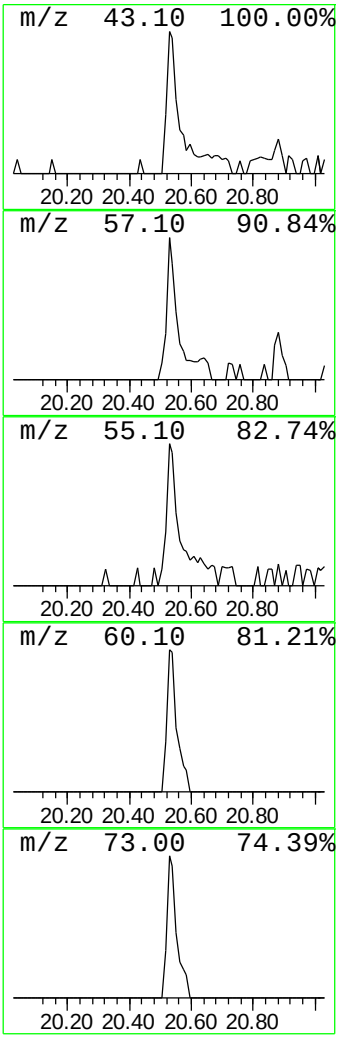
Peak Number 6 Dodecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.53	2.59 ng	52988	Phenanthrene-d10	18.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	64
2	Undecanoic acid	186	C11H22O2	000112-37-8	59
3	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	50
4	n-Decanoic acid	172	C10H20O2	000334-48-5	50
5	.alpha.-D-Glucopyranoside, .alph...	342	C12H22O11	000099-20-7	43





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091115\
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Operator : UM/IZ
Sample : G3558-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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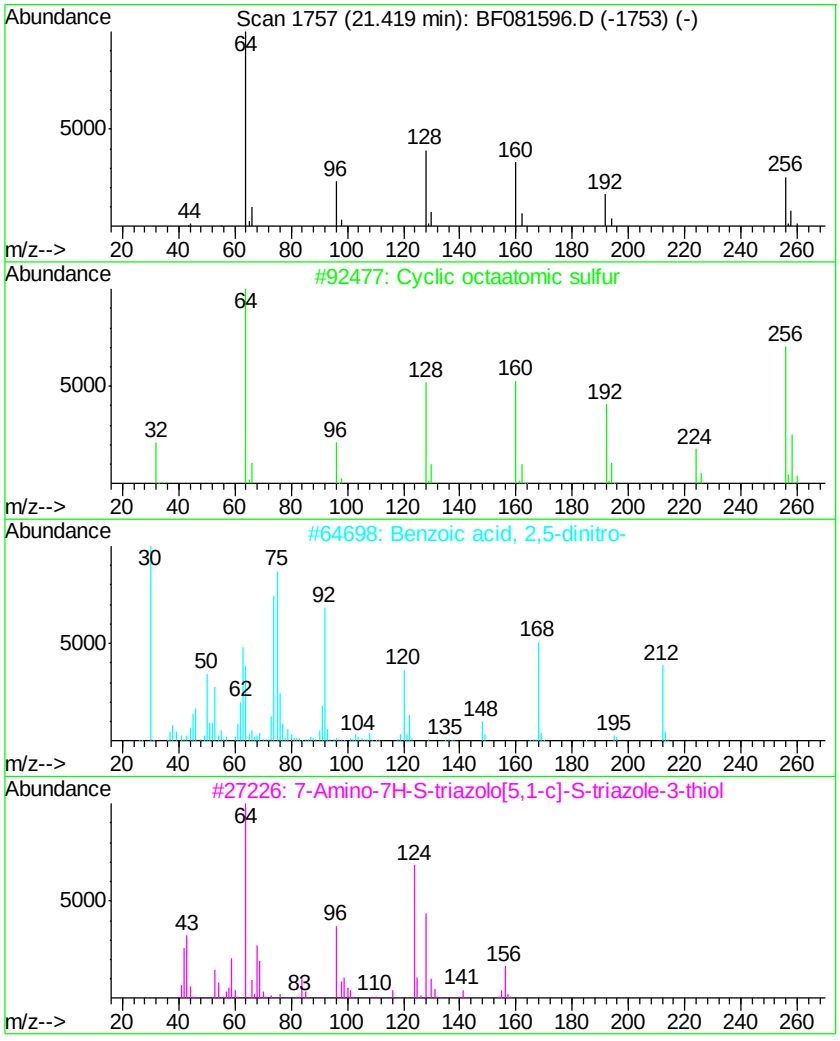
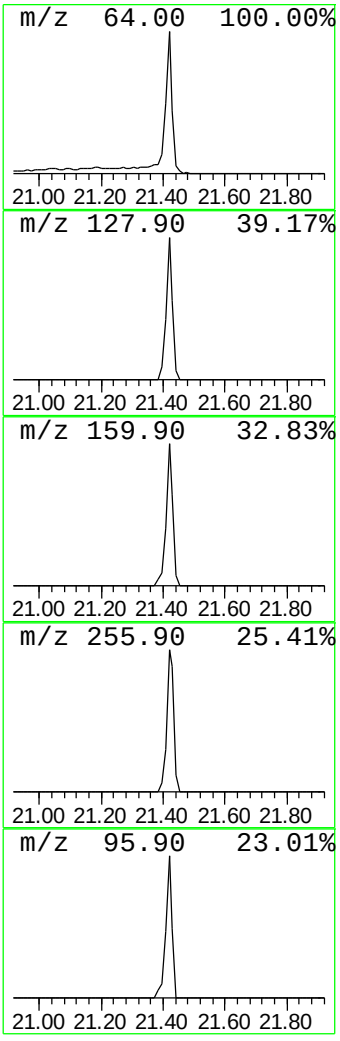
Peak Number 7 Cyclic octaatomic sulfur Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.42	6.80 ng	121784	Chrysene-d12	23.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclic octaatomic sulfur	256	S8	010544-50-0	95
2	Benzoic acid, 2,5-dinitro-	212	C7H4N2O6	000610-28-6	53
3	7-Amino-7H-S-triazolo[5,1-c]-S-t...	156	C3H4N6S	013728-28-4	39
4	Dihydropyrimidine-2-methyl thios...	208	C5H8N2O3S2	1000256-28-8	9
5	1,2,5,6-Tetrathiocane	184	C4H8S4	001940-01-8	9





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Data File : BF081596.D
Acq On : 11 Sep 2015 22:24
Operator : UM/IZ
Sample : G3558-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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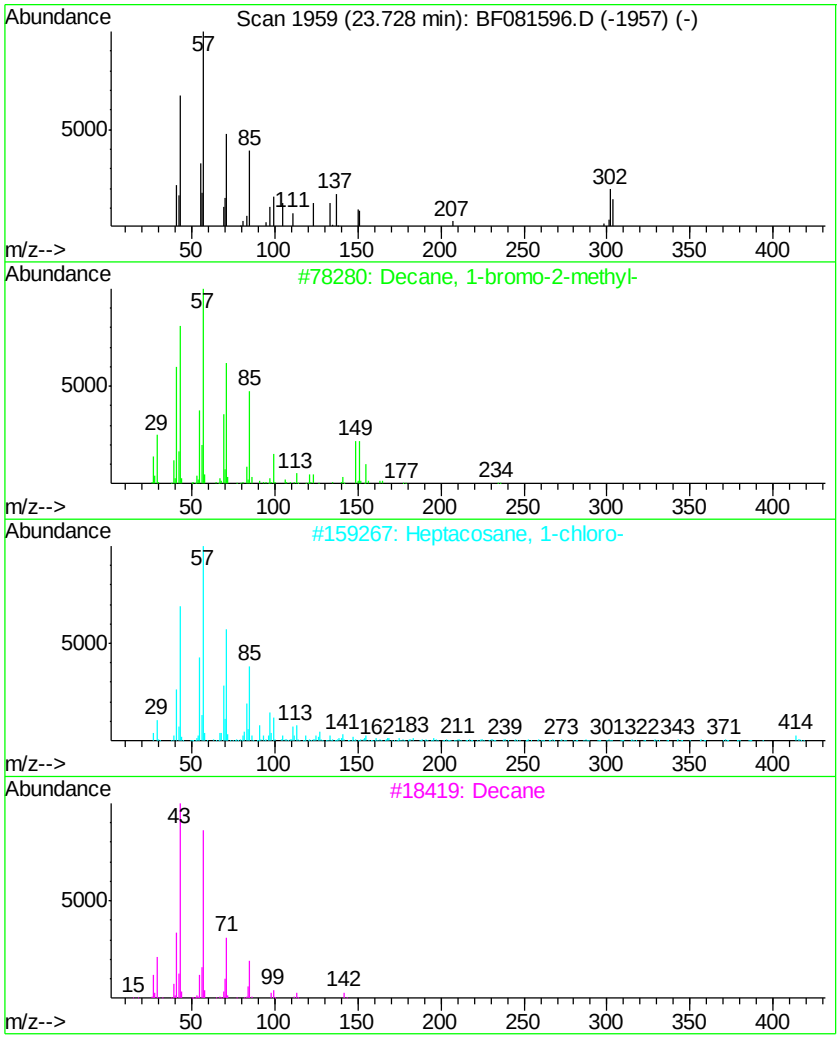
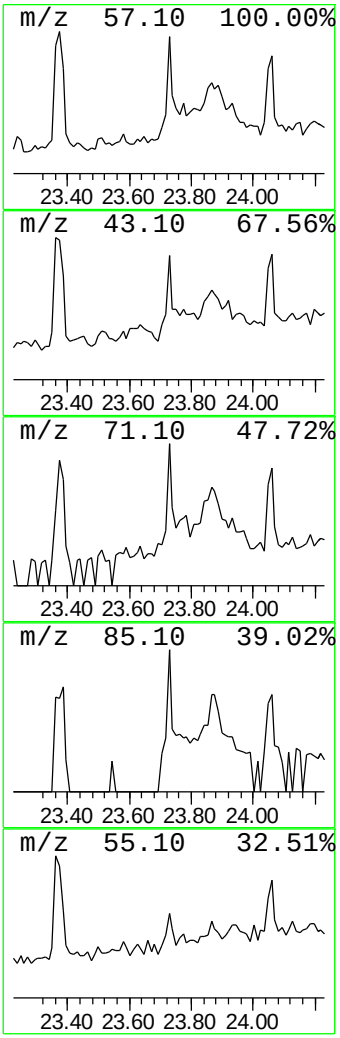
Peak Number 8 unknown23.73 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.73	2.00 ng	35901	Chrysene-d12	23.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 1-bromo-2-methyl-	234	C11H23Br	127839-47-8	43
2	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	43
3	Decane	142	C10H22	000124-18-5	43
4	Dodecane, 2-methyl-	184	C13H28	001560-97-0	43
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	43





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Data File : BF081596.D
Acq On : 11 Sep 2015 22:24
Operator : UM/IZ
Sample : G3558-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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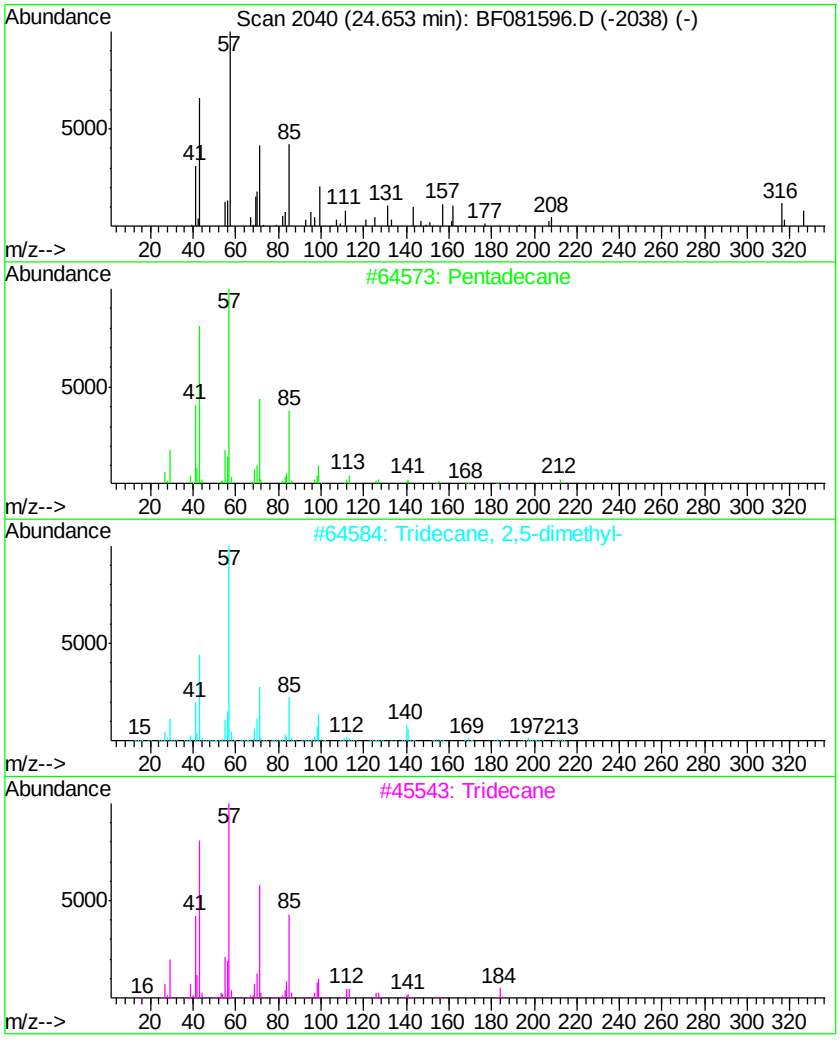
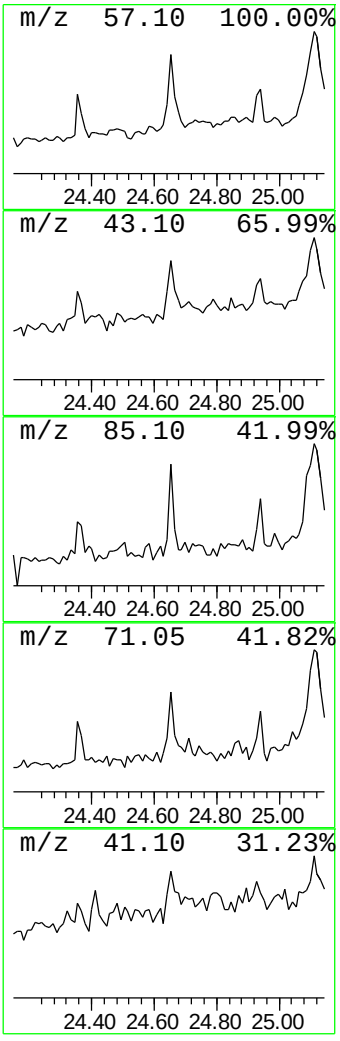
Peak Number 10 unknown24.65 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.65	2.42 ng	31642	Perylene-d12	24.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	38
2	Tridecane, 2,5-dimethyl-	212	C15H32	056292-66-1	38
3	Tridecane	184	C13H28	000629-50-5	38
4	Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	38
5	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091115\
Data File : BF081596.D
Acq On : 11 Sep 2015 22:24
Operator : UM/IZ
Sample : G3558-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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
Manganese(II) ace...	1.46	3.7	ng	62951	1	8.25	339388	20.0
2-Pentanone, 4-hy...	4.56	57.4	ng	974693	1	8.25	339388	20.0
unknown7.77	7.77	97.2	ng	1649140	1	8.25	339388	20.0
Dodecanoic acid	20.53	2.6	ng	52988	4	18.79	409039	20.0
Cyclic octaatomic...	21.42	6.8	ng	121784	5	23.40	358369	20.0
unknown23.73	23.73	2.0	ng	35901	5	23.40	358369	20.0
unknown24.65	24.65	2.4	ng	31642	6	24.84	261065	20.0