LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091415\
Data File : BF081613.D
Acq On : 14 Sep 2015 18:14
Operator : UM/IZ
Sample : G3597-07 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-7(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-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	1.462	8	11	16	rBV	48251	132498	5.57%	0.930%
2	1.542	16	18	57	rVB	682863	2377214	100.00%	16.691%
3	4.503	273	277	293	rBV	207964	512508	21.56%	3.599%
4	5.383	351	354	374	rBB	456295	859385	36.15%	6.034%
5	7.646	549	552	558	rBV	520554	907877	38.19%	6.375%
6	7.749	558	561	571	rVB	549696	929367	39.09%	6.525%
7	8.229	600	603	609	rBB	232424	366133	15.40%	2.571%
8	8.560	628	632	635	rBV	390088	648500	27.28%	4.553%
9	9.520	712	716	725	rBV	323777	582091	24.49%	4.087%
10	11.132	853	857	861	rBV	304875	467113	19.65%	3.280%
11	13.772	1084	1088	1091	rBV	575345	941984	39.63%	6.614%
12	14.824	1177	1180	1184	rBV	92288	149196	6.28%	1.048%
13	15.270	1215	1219	1223	rBV	291056	469631	19.76%	3.297%
14	16.664	1338	1341	1344	rBV	17346	29416	1.24%	0.207%
15	17.167	1381	1385	1391	rBV	311493	514439	21.64%	3.612%
16	17.807	1436	1441	1448	rBV	20027	56266	2.37%	0.395%
17	18.778	1522	1526	1528	rBV	233909	421801	17.74%	2.962%
18	18.824	1528	1530	1533	rVV	53288	79708	3.35%	0.560%
19	18.893	1533	1536	1539	rVV2	20177	35584	1.50%	0.250%
20	18.950	1539	1541	1550	rVB2	18518	37272	1.57%	0.262%
21	19.933	1623	1627	1630	rBV	16962	32326	1.36%	0.227%
22	20.241	1650	1654	1657	rVV2	12773	35919	1.51%	0.252%
23	20.527	1676	1679	1686	rBV	34513	81210	3.42%	0.570%
24	20.756	1694	1699	1702	rBV4	9793	25241	1.06%	0.177%
25	20.870	1706	1709	1712	rBV	19030	26472	1.11%	0.186%
26	21.213	1736	1739	1741	rBV	20119	36853	1.55%	0.259%
27	21.442	1756	1759	1761	rBV	149710	188611	7.93%	1.324%
28	21.567	1765	1770	1772	rBV3	19204	40164	1.69%	0.282%
29	21.784	1786	1789	1793	rBV	176492	271226	11.41%	1.904%
30	21.910	1797	1800	1803	rBV2	22170	42703	1.80%	0.300%
31	22.036	1809	1811	1813	rBV	104734	130960	5.51%	0.920%
32	22.116	1816	1818	1820	rBV	497043	615444	25.89%	4.321%
33	22.150	1820	1821	1824	rVB2	29637	42578	1.79%	0.299%
34	22.276	1829	1832	1833	rBV2	18160	40412	1.70%	0.284%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091415\
Data File : BF081613.D
Acq On : 14 Sep 2015 18:14
Operator : UM/IZ
Sample : G3597-07 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-7(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-BF090115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	22.436	1844	1846	1850	rVV2	33884	57444	2.42%	0.403%
36	22.550	1854	1856	1858	rVV	34465	42261	1.78%	0.297%
37	22.585	1858	1859	1861	rVB2	31195	40478	1.70%	0.284%
38	22.950	1888	1891	1894	rBV2	81604	147329	6.20%	1.034%
39	23.087	1902	1903	1905	rVV2	25308	38179	1.61%	0.268%
40	23.133	1905	1907	1910	rVB2	23819	44406	1.87%	0.312%
41	23.225	1913	1915	1918	rVV	30152	37713	1.59%	0.265%
42	23.396	1925	1930	1931	rBV2	329658	580244	24.41%	4.074%
43	23.419	1931	1932	1934	rVB	128247	132128	5.56%	0.928%
44	23.499	1937	1939	1941	rVB2	26880	32457	1.37%	0.228%
45	23.727	1957	1959	1961	rBV2	28816	42180	1.77%	0.296%
46	23.842	1966	1969	1971	rBV	45539	55622	2.34%	0.391%
47	24.048	1985	1987	1990	rVB3	27922	43759	1.84%	0.307%
48	24.356	2012	2014	2016	rBV2	28556	32295	1.36%	0.227%
49	24.493	2024	2026	2029	rBV	120550	192800	8.11%	1.354%
50	24.653	2038	2040	2041	rBV	30394	42561	1.79%	0.299%
51	24.733	2045	2047	2049	rVV	95791	113371	4.77%	0.796%
52	24.779	2049	2051	2053	rVV	104651	121530	5.11%	0.853%
53	24.836	2053	2056	2062	rVV	163520	317262	13.35%	2.228%

Sum of corrected areas: 14242121

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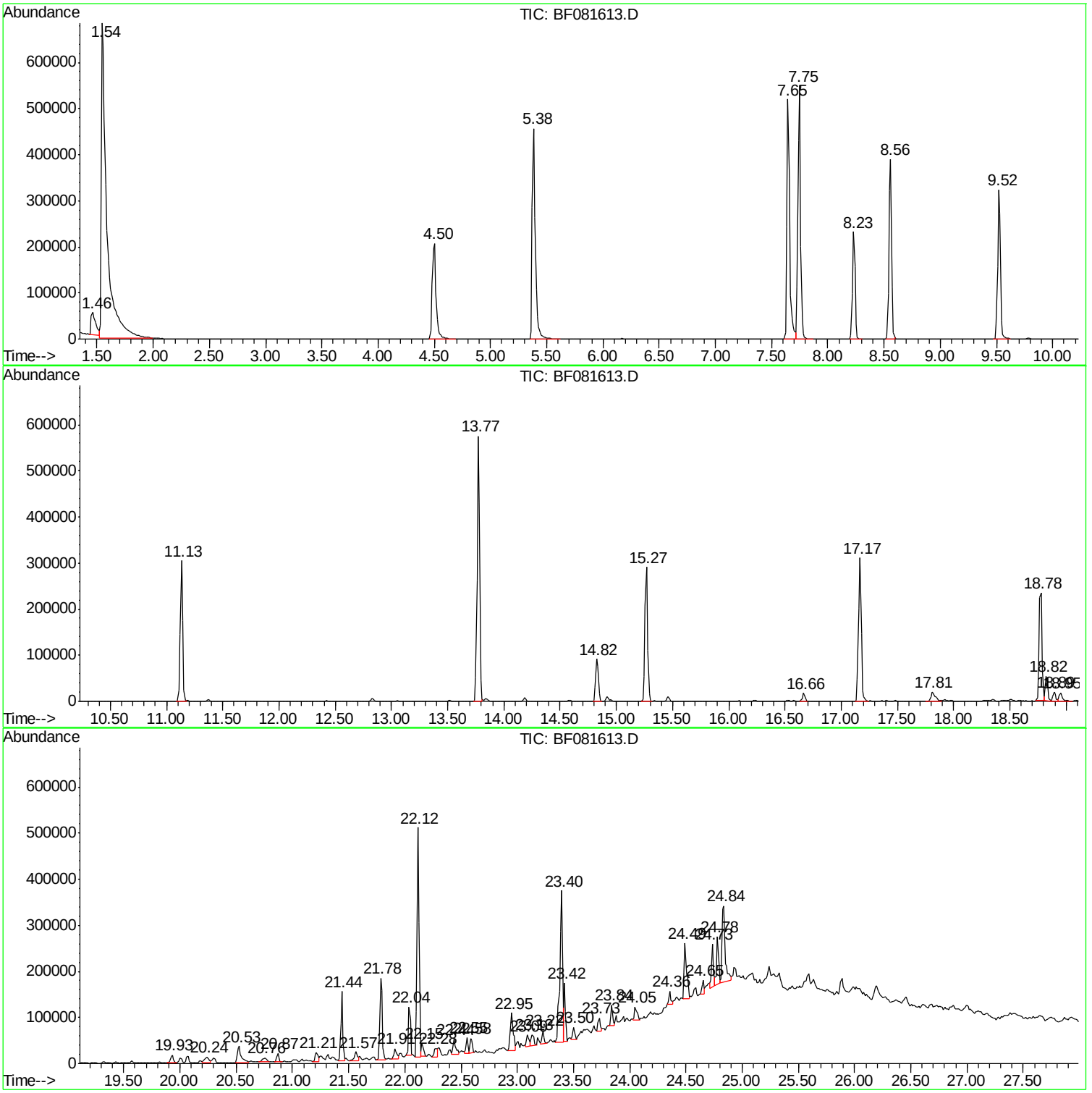
Acq On : 14 Sep 2015 18:14
Operator : UM/IZ
Sample : G3597-07 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GP-7(0-5)

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\BF091415\
Data File : BF081613.D
Acq On : 14 Sep 2015 18:14
Operator : UM/IZ
Sample : G3597-07 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-7(0-5)

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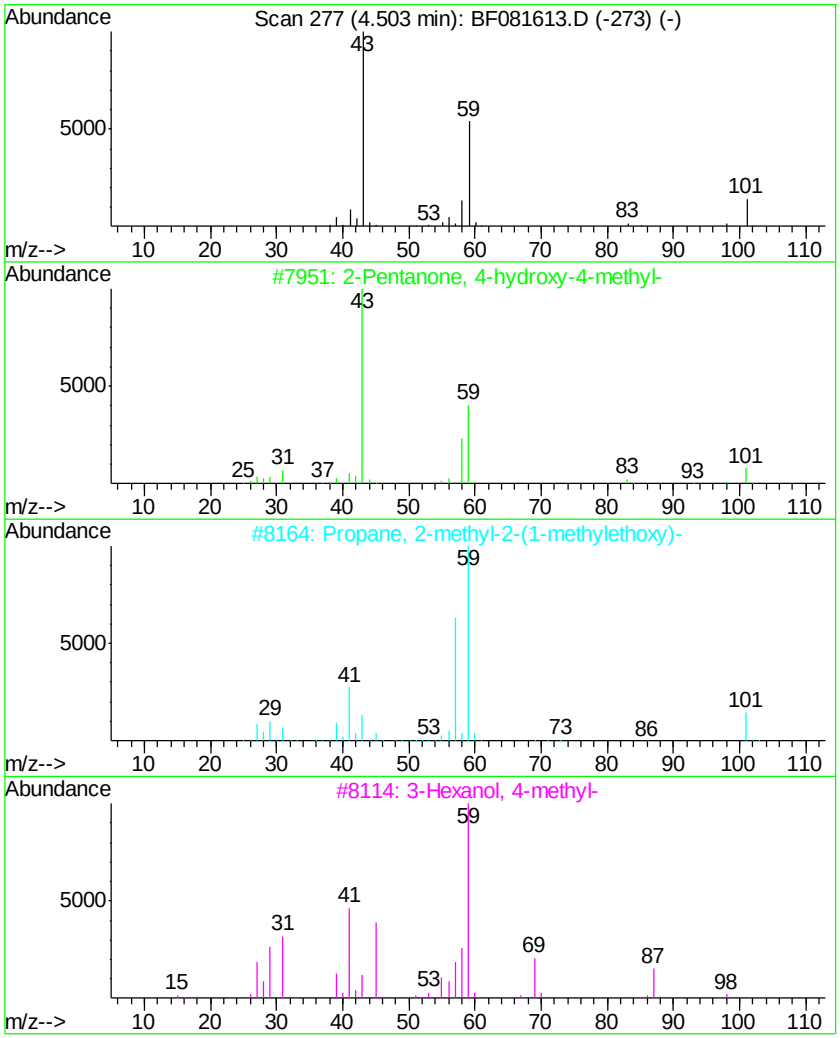
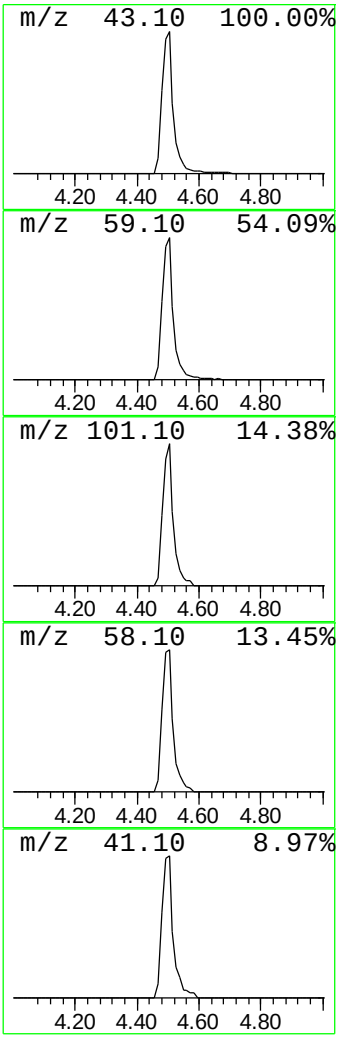
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.50	28.00 ng	512508	1,4-Dichlorobenzene-d4	8.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
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	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091415\
Data File : BF081613.D
Acq On : 14 Sep 2015 18:14
Operator : UM/IZ
Sample : G3597-07 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-7(0-5)

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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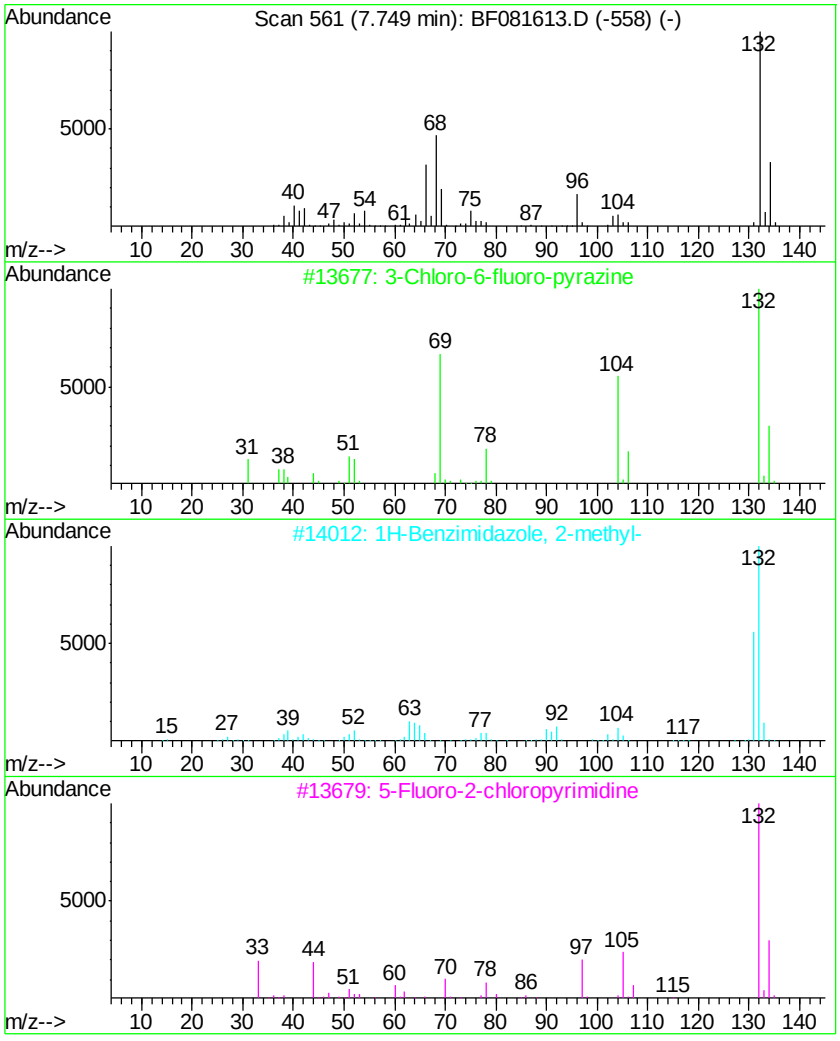
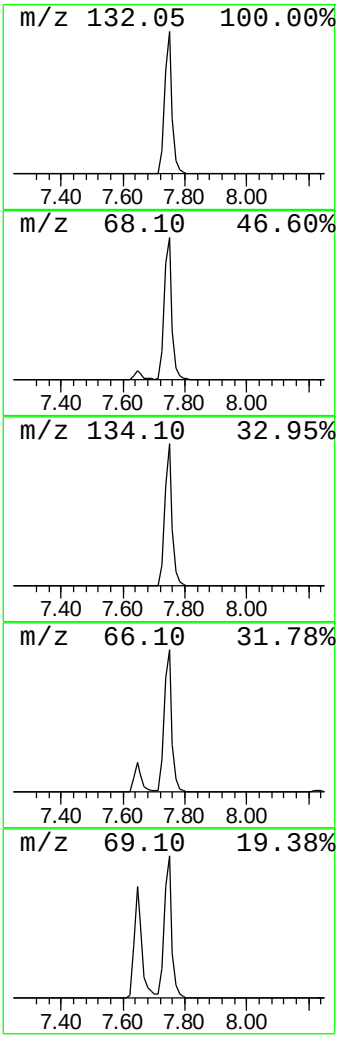
Peak Number 4 unknown7.75 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.75	50.77 ng	929367	1,4-Dichlorobenzene-d4	8.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091415\
Data File : BF081613.D
Acq On : 14 Sep 2015 18:14
Operator : UM/IZ
Sample : G3597-07 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-7(0-5)

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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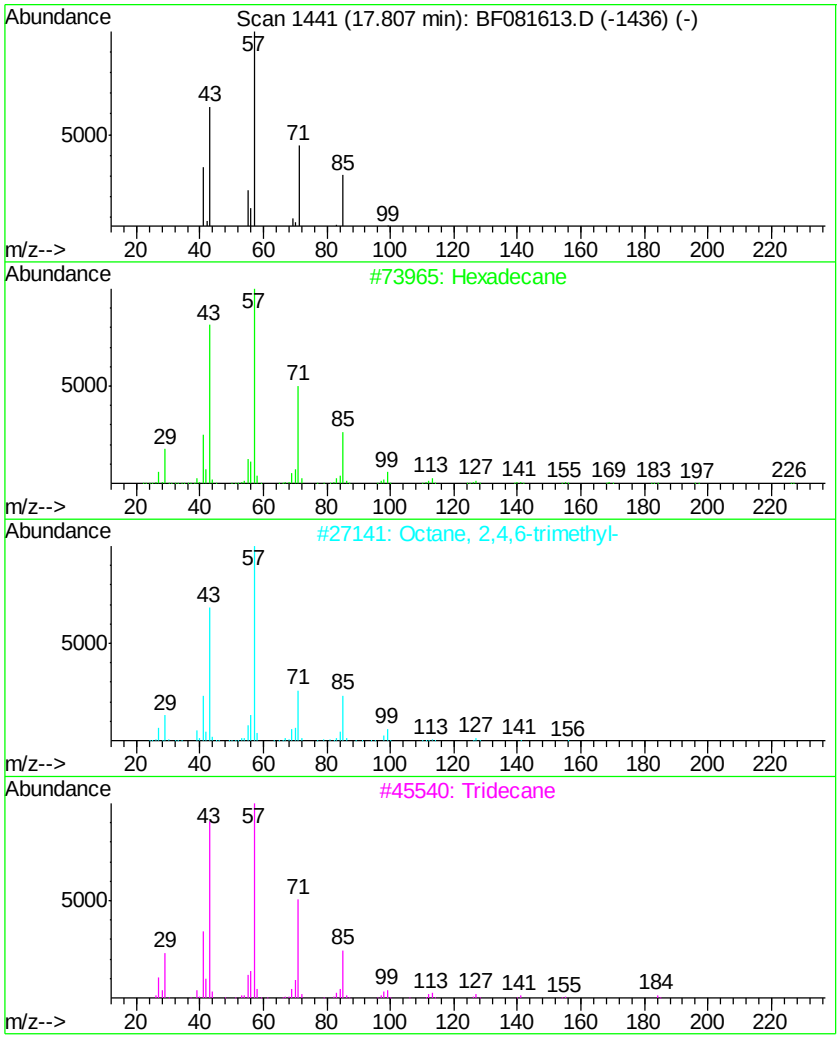
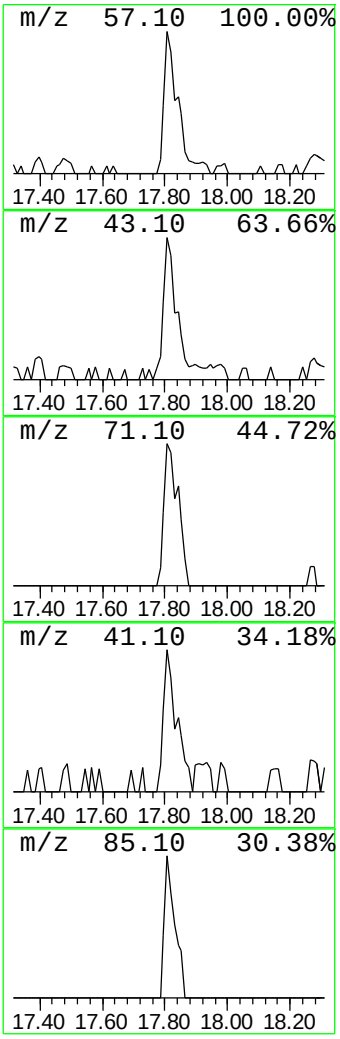
Peak Number 6 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.81	2.67 ng	56266	Phenanthrene-d10	18.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	83
2	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	83
3	Tridecane	184	C13H28	000629-50-5	64
4	Ether, hexyl pentyl	172	C11H24O	032357-83-8	53
5	Hexane, 2,2,3,3-tetramethyl-	142	C10H22	013475-81-5	50





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091415\
Data File : BF081613.D
Acq On : 14 Sep 2015 18:14
Operator : UM/IZ
Sample : G3597-07 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-7(0-5)

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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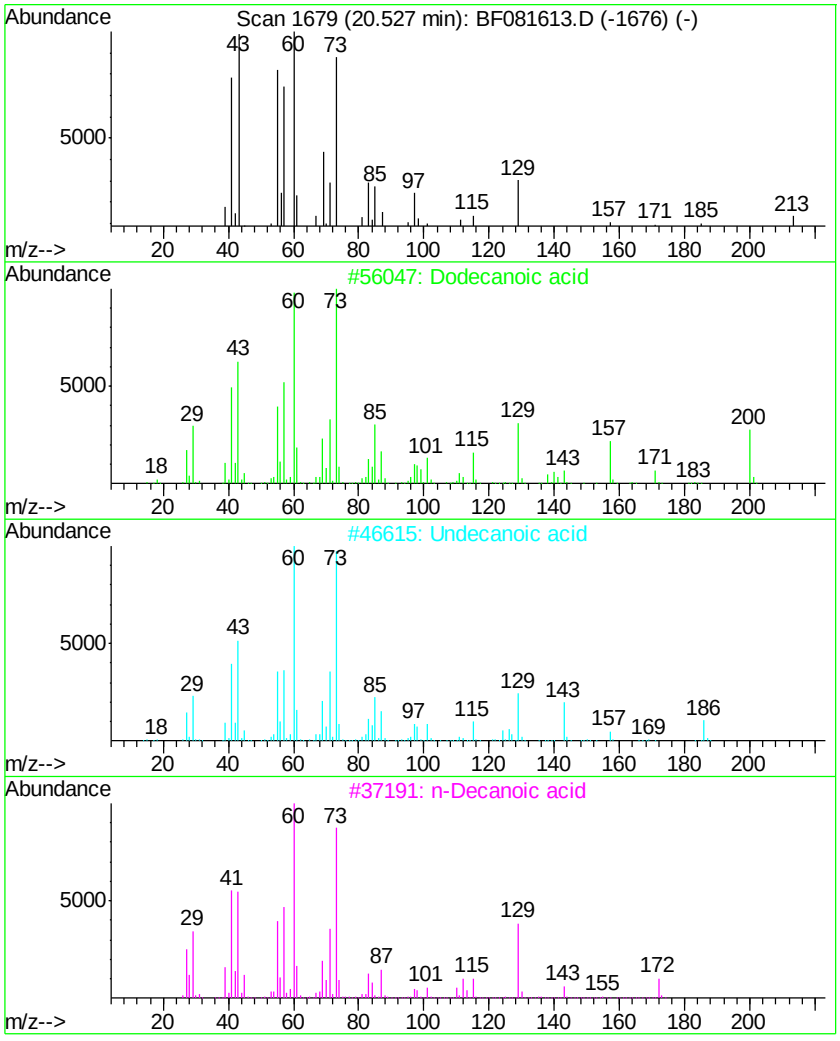
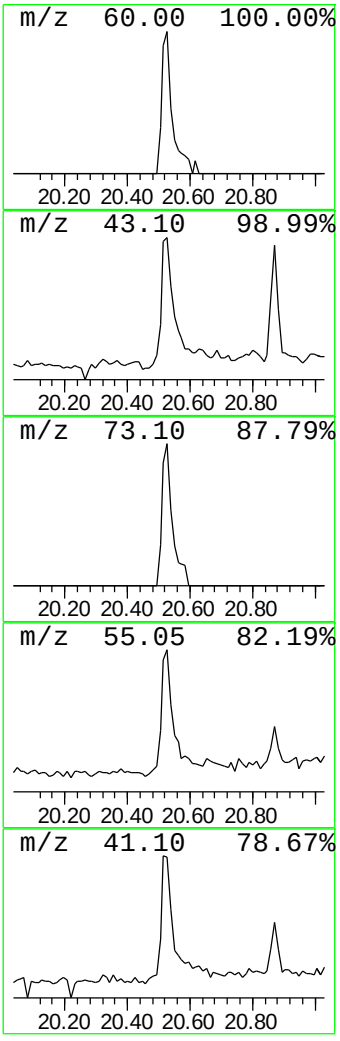
Peak Number 7 Dodecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.53	3.85 ng	81210	Phenanthrene-d10	18.78

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	58
3	n-Decanoic acid	172	C10H20O2	000334-48-5	47
4	d-Glucohexodialdose	178	C6H10O6	1000149-19-1	43
5	.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	40





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091415\
Data File : BF081613.D
Acq On : 14 Sep 2015 18:14
Operator : UM/IZ
Sample : G3597-07 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-7(0-5)

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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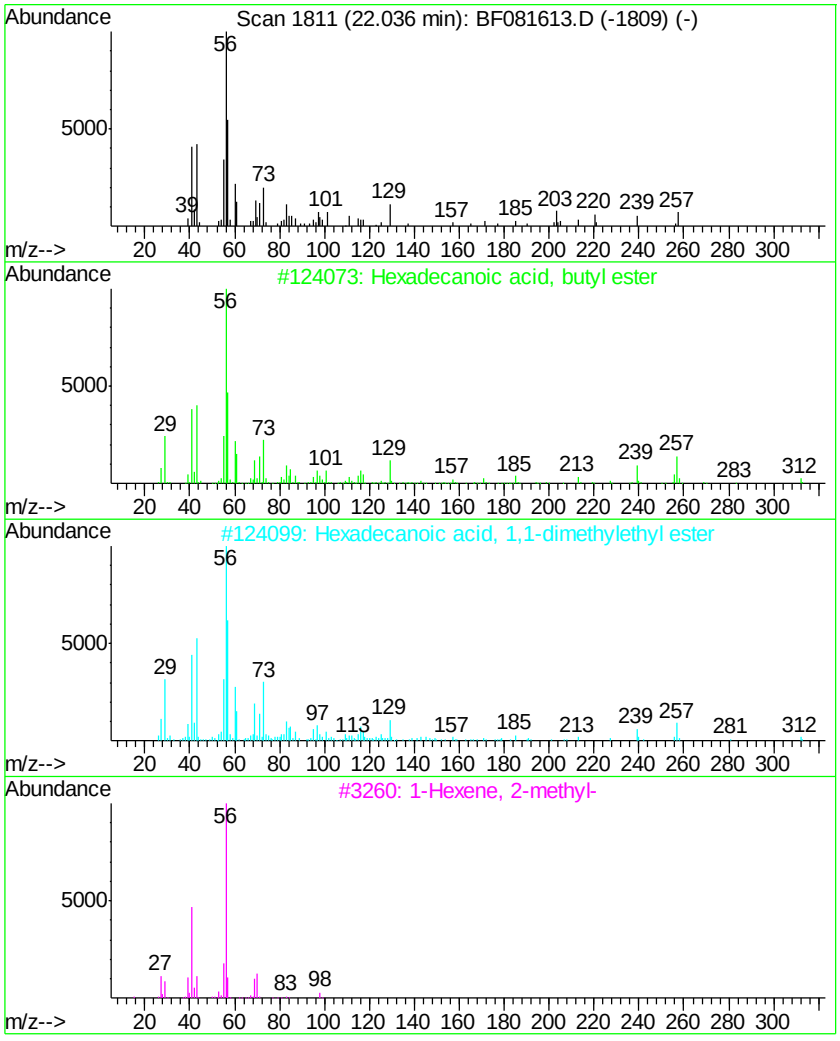
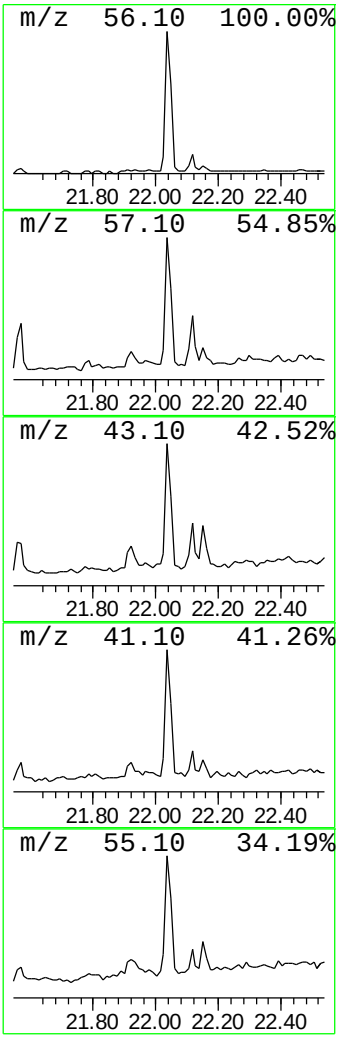
Peak Number 8 Hexadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.04	4.51 ng	130960	Chrysene-d12	23.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	72
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	47
3	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	35
4	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35
5	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091415\
Data File : BF081613.D
Acq On : 14 Sep 2015 18:14
Operator : UM/IZ
Sample : G3597-07 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-7(0-5)

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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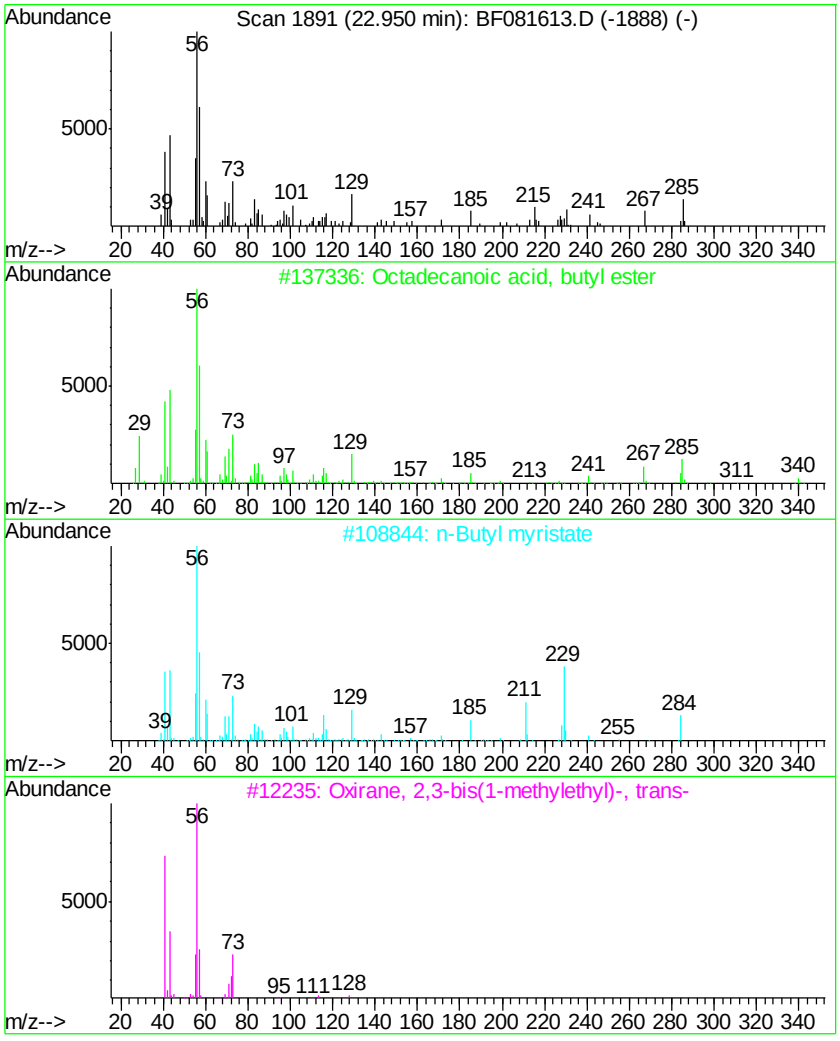
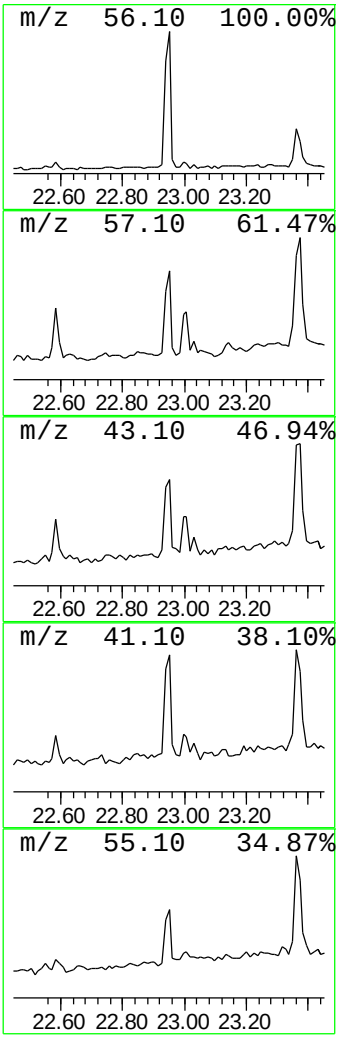
Peak Number 9 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.95	5.08 ng	147329	Chrysene-d12	23.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	90
2	n-Butyl myristate	284	C18H36O2	000110-36-1	83
3	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	46
4	Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	35
5	Cyclopentanone, 2,2-dimethyl-	112	C7H12O	004541-32-6	27





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091415\
Data File : BF081613.D
Acq On : 14 Sep 2015 18:14
Operator : UM/IZ
Sample : G3597-07 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-7(0-5)

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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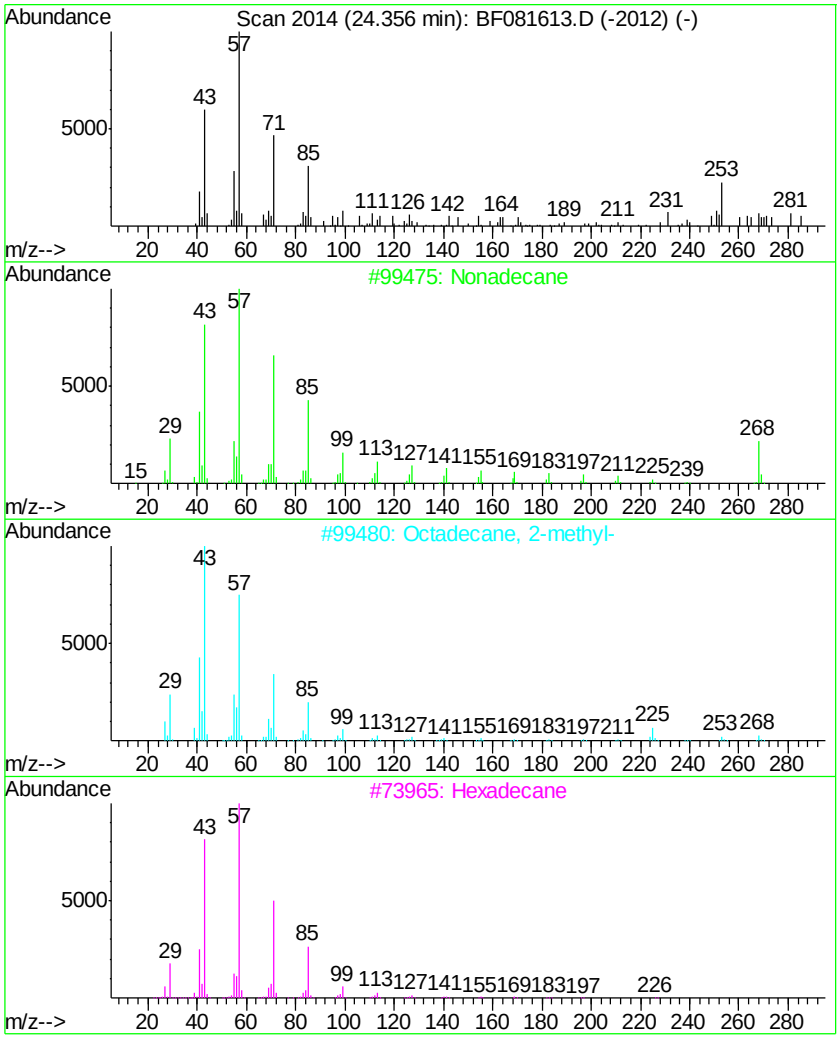
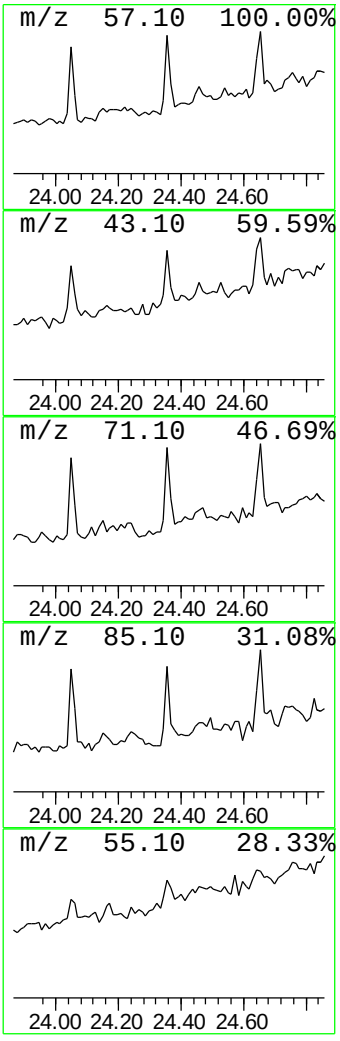
Peak Number 10 unknown24.36 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.36	2.04 ng	32295	Perylene-d12	24.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	43
2	Octadecane, 2-methyl-	268	C19H40	001560-88-9	43
3	Hexadecane	226	C16H34	000544-76-3	38
4	Dodecane	170	C12H26	000112-40-3	38
5	Dodecane, 3-methyl-	184	C13H28	017312-57-1	38





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091415\
Data File : BF081613.D
Acq On : 14 Sep 2015 18:14
Operator : UM/IZ
Sample : G3597-07 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-7(0-5)

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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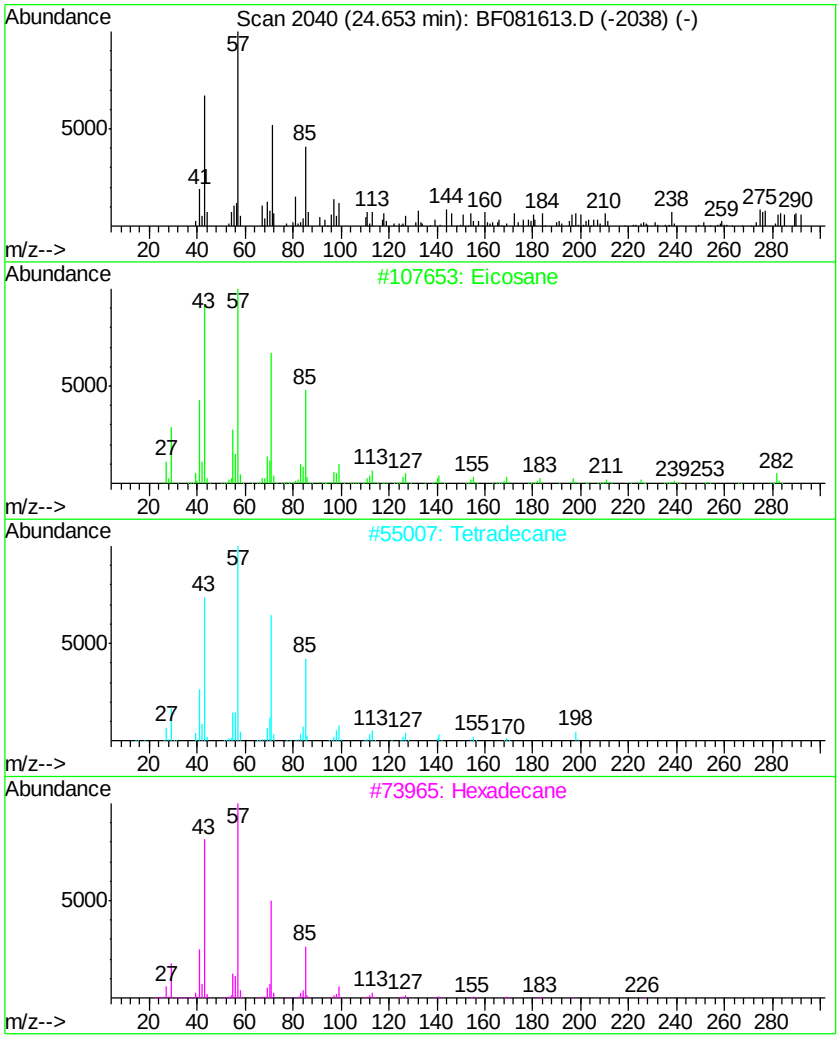
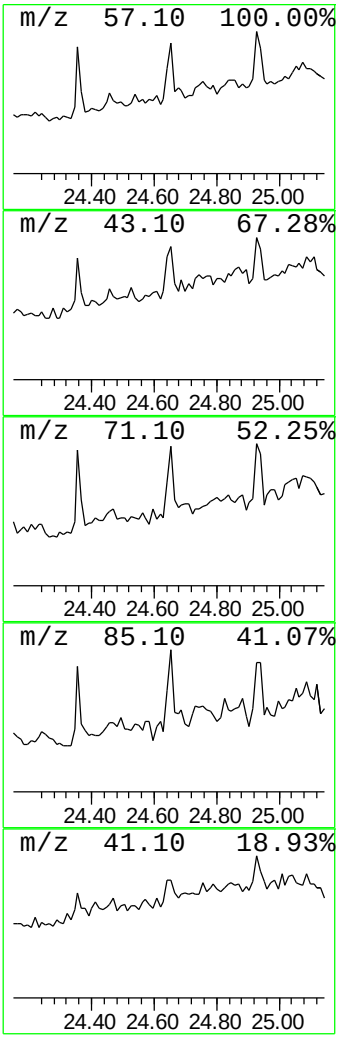
Peak Number 11 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.65	2.68 ng	42561	Perylene-d12	24.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	86
2	Tetradecane	198	C14H30	000629-59-4	83
3	Hexadecane	226	C16H34	000544-76-3	64
4	Tridecane	184	C13H28	000629-50-5	58
5	Dodecane, 3-methyl-	184	C13H28	017312-57-1	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091415\
Data File : BF081613.D
Acq On : 14 Sep 2015 18:14
Operator : UM/IZ
Sample : G3597-07 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-7(0-5)

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
2-Pentanone, 4-hy...	4.50	28.0	ng	512508	1	8.23	366133	20.0
unknown7.75	7.75	50.8	ng	929367	1	8.23	366133	20.0
Hexadecane	17.81	2.7	ng	56266	4	18.78	421801	20.0
Dodecanoic acid	20.53	3.9	ng	81210	4	18.78	421801	20.0
Hexadecanoic acid...	22.04	4.5	ng	130960	5	23.40	580244	20.0
Octadecanoic acid...	22.95	5.1	ng	147329	5	23.40	580244	20.0
unknown24.36	24.36	2.0	ng	32295	6	24.84	317262	20.0
Eicosane	24.65	2.7	ng	42561	6	24.84	317262	20.0