LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081663.D
Acq On : 17 Sep 2015 3:01
Operator : UM/IZ
Sample : G3624-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-SOURCE-6

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	1.451	7	10	15	rBV	35783	101672	4.90%	0.549%
2	1.531	15	17	52	rVB	185506	634108	30.54%	3.422%
3	4.491	271	276	293	rBV	335168	1079688	52.01%	5.827%
4	5.349	348	351	371	rBV	921003	1829311	88.11%	9.872%
5	7.612	544	549	553	rBV	936592	1841266	88.69%	9.937%
6	7.703	553	557	560	rVB	1069506	1867387	89.95%	10.078%
7	8.183	596	599	604	rBB	210479	326734	15.74%	1.763%
8	8.515	623	628	631	rBV	796108	1364988	65.75%	7.366%
9	9.486	708	713	716	rBV	620368	1211130	58.34%	6.536%
10	11.075	849	852	857	rBV	229625	419733	20.22%	2.265%
11	13.727	1079	1084	1087	rBV	1033729	2076064	100.00%	11.204%
12	14.778	1172	1176	1185	rBV	204692	341356	16.44%	1.842%
13	15.212	1210	1214	1219	rBB	262362	443652	21.37%	2.394%
14	16.618	1333	1337	1340	rBB	14952	27518	1.33%	0.149%
15	17.121	1376	1381	1391	rBB	663694	1274952	61.41%	6.881%
16	17.750	1432	1436	1442	rBV	21579	53204	2.56%	0.287%
17	18.710	1516	1520	1527	rBV	269598	466859	22.49%	2.519%
18	18.836	1527	1531	1534	rBV2	19854	33898	1.63%	0.183%
19	19.864	1617	1621	1625	rBB	10724	21243	1.02%	0.115%
20	20.470	1671	1674	1686	rVB2	53295	107070	5.16%	0.578%
21	21.876	1795	1797	1803	rBV	13284	23336	1.12%	0.126%
22	22.082	1811	1815	1818	rBV	1430911	1933007	93.11%	10.432%
23	23.350	1920	1926	1929	rBV	410586	532394	25.64%	2.873%
24	24.013	1981	1984	1990	rBV2	25290	44326	2.14%	0.239%
25	24.368	2013	2015	2017	rVB	19156	23880	1.15%	0.129%
26	24.608	2034	2036	2038	rBV	35172	43682	2.10%	0.236%
27	24.790	2049	2052	2055	rBV	248897	262950	12.67%	1.419%
28	24.893	2058	2061	2063	rBV2	14587	21856	1.05%	0.118%
29	25.190	2084	2087	2089	rBV	24861	31998	1.54%	0.173%
30	25.248	2089	2092	2098	rVB3	12408	36090	1.74%	0.195%
31	26.231	2174	2178	2182	rBV3	12118	33722	1.62%	0.182%
32	26.894	2233	2236	2242	rVB5	5354	20833	1.00%	0.112%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081663.D
Acq On : 17 Sep 2015 3:01
Operator : UM/IZ
Sample : G3624-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-SOURCE-6

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

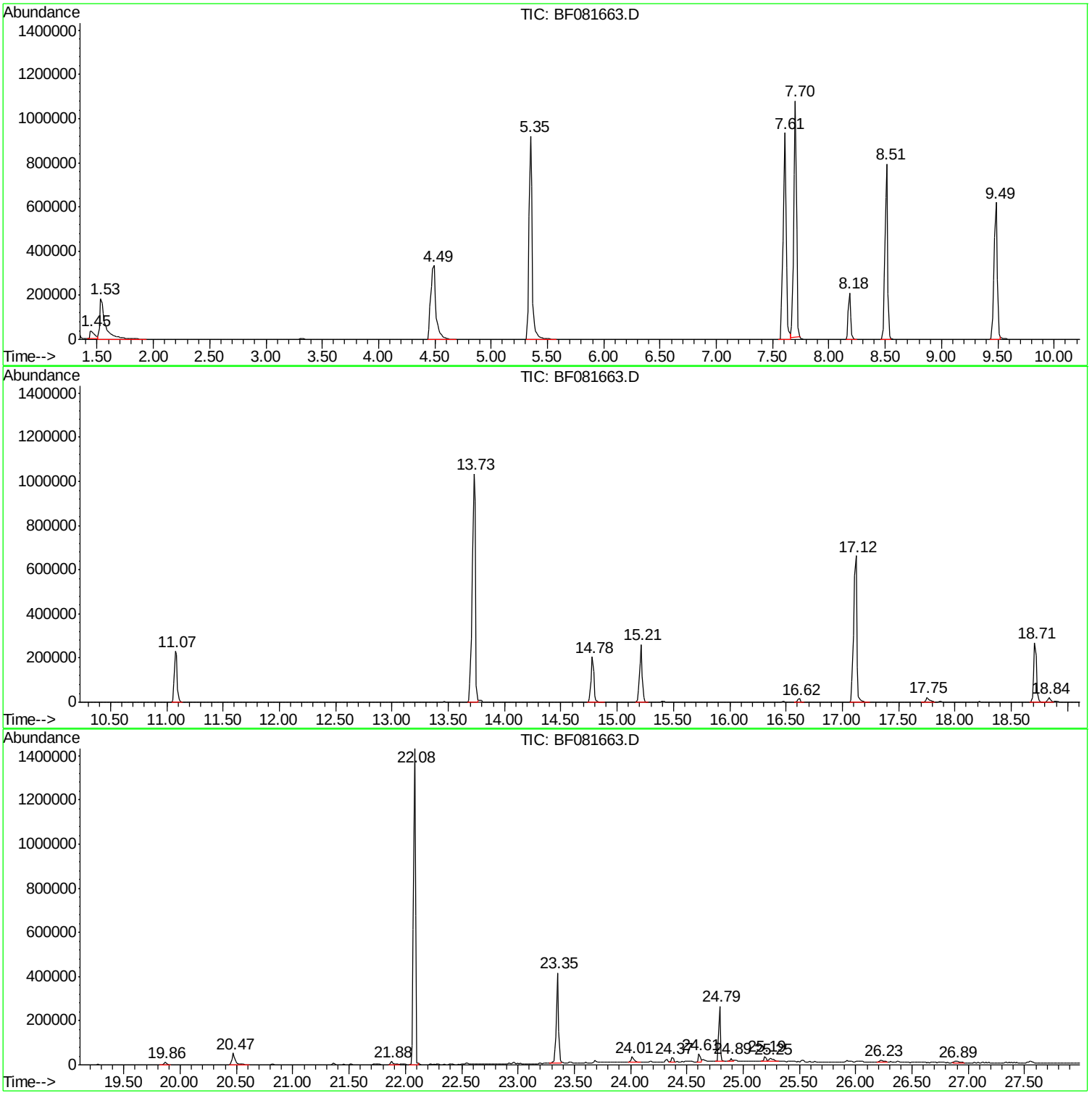
Sum of corrected areas: 18529907

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081663.D
Acq On : 17 Sep 2015 3:01
Operator : UM/IZ
Sample : G3624-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-SOURCE-6

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\BF091615\
Data File : BF081663.D
Acq On : 17 Sep 2015 3:01
Operator : UM/IZ
Sample : G3624-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-SOURCE-6

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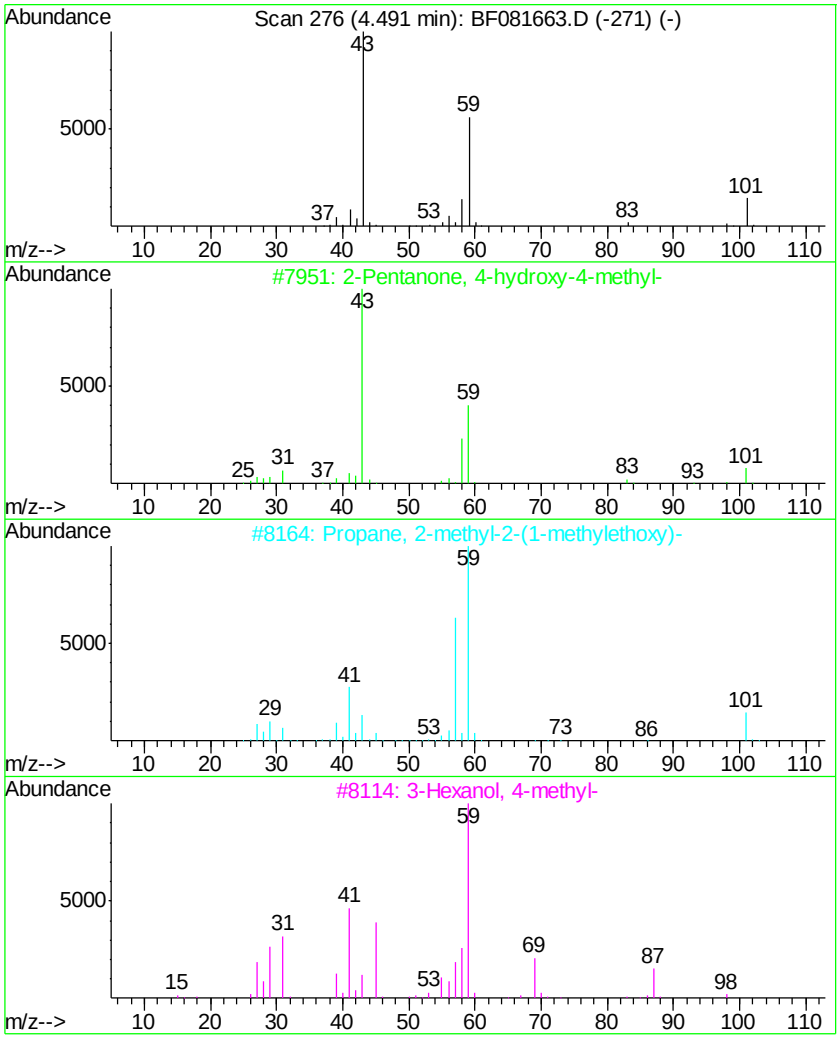
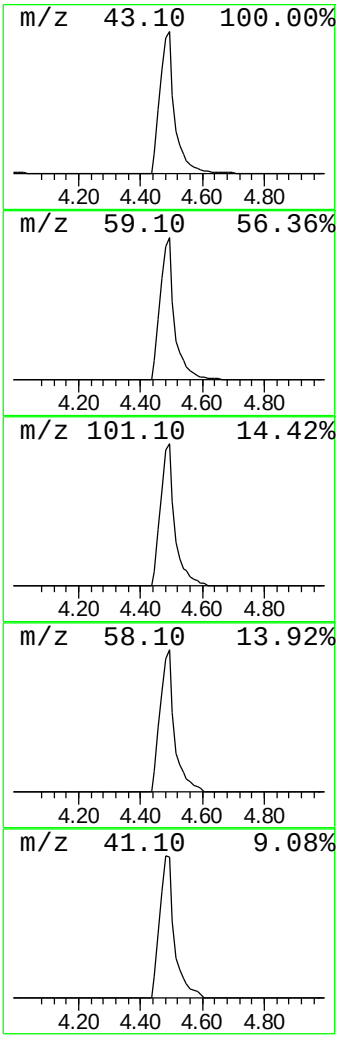
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.49	66.09 ng	1079690	1,4-Dichlorobenzene-d4	8.18

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	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081663.D
Acq On : 17 Sep 2015 3:01
Operator : UM/IZ
Sample : G3624-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-SOURCE-6

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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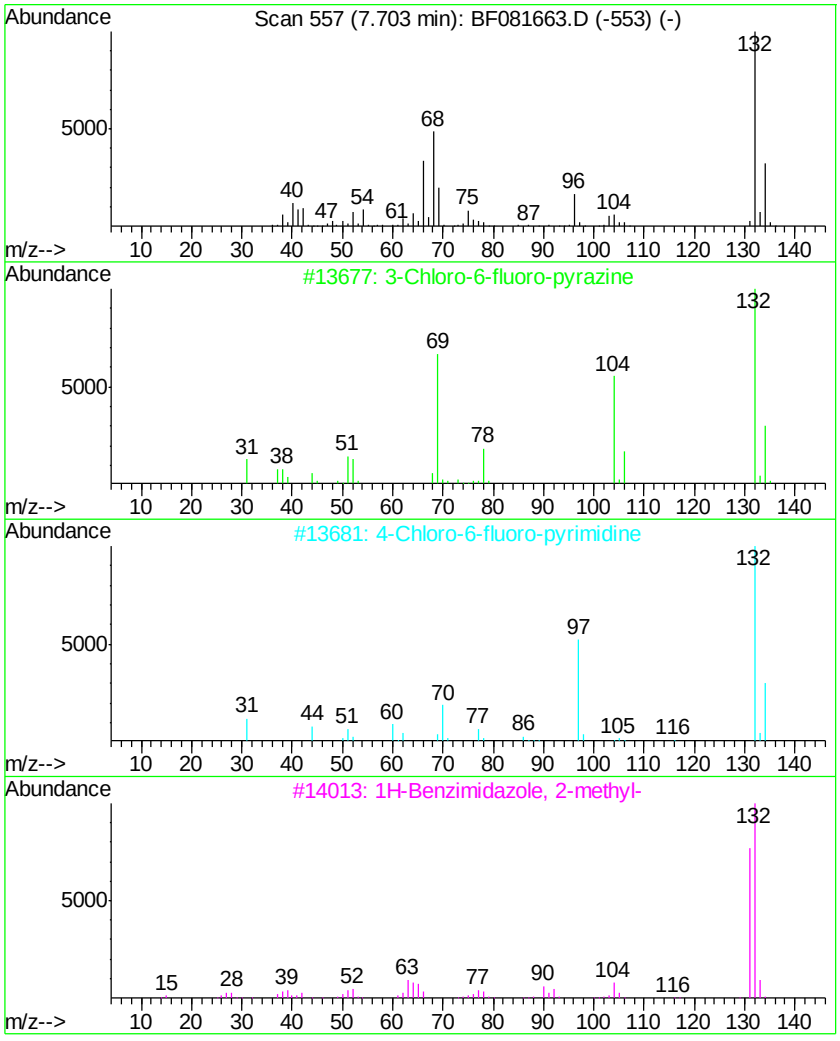
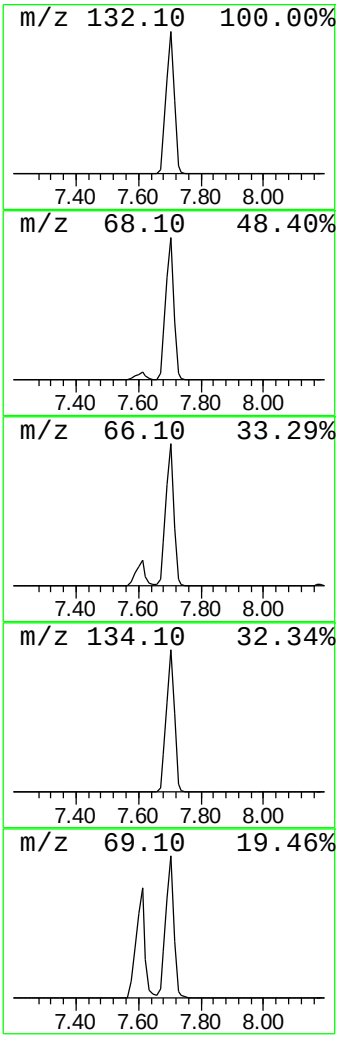
Peak Number 4 unknown7.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	114.31 ng	1867390	1,4-Dichlorobenzene-d4	8.18

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	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081663.D
Acq On : 17 Sep 2015 3:01
Operator : UM/IZ
Sample : G3624-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-SOURCE-6

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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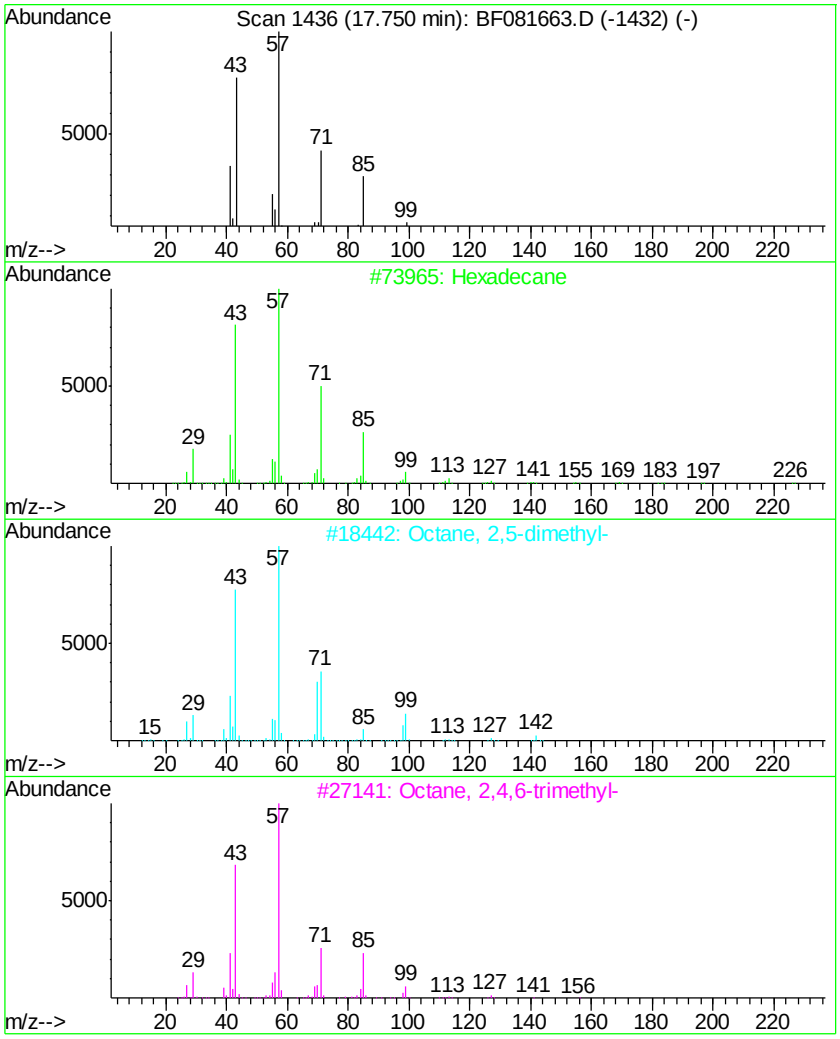
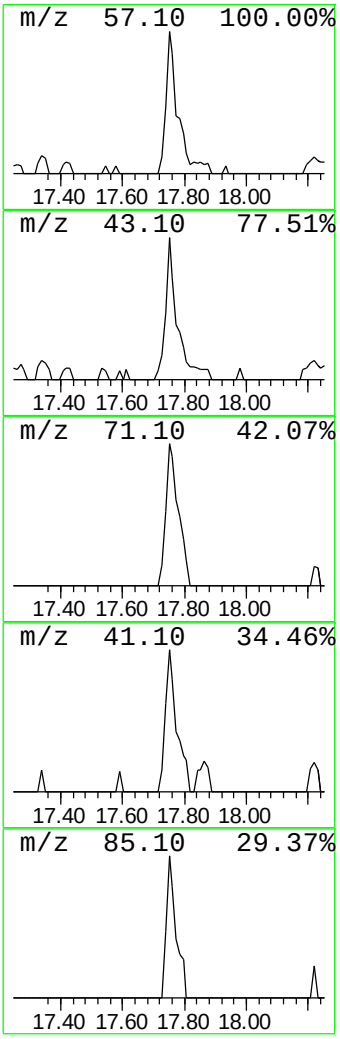
Peak Number 6 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.75	2.28 ng	53204	Phenanthrene-d10	18.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	83
2	Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	64
3	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	64
4	Tridecane	184	C13H28	000629-50-5	64
5	Ether, hexyl pentyl	172	C11H24O	032357-83-8	59





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081663.D
Acq On : 17 Sep 2015 3:01
Operator : UM/IZ
Sample : G3624-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-SOURCE-6

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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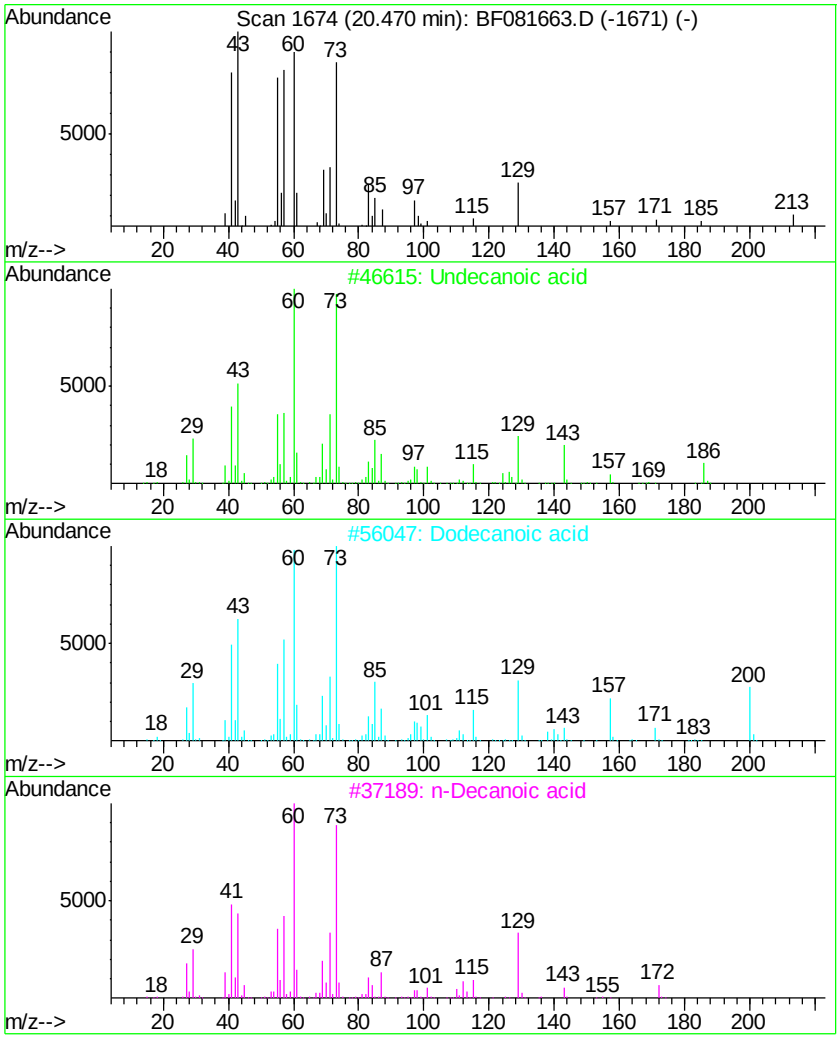
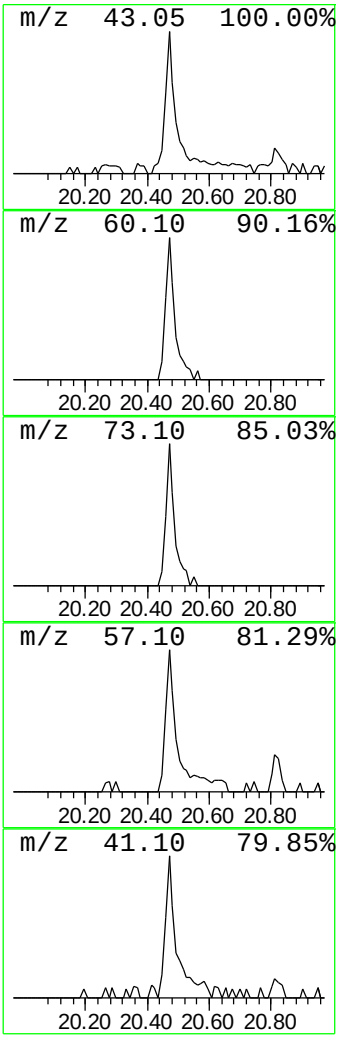
Peak Number 7 Undecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.47	4.59 ng	107070	Phenanthrene-d10	18.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	80
2	Dodecanoic acid	200	C12H24O2	000143-07-7	59
3	n-Decanoic acid	172	C10H20O2	000334-48-5	53
4	Nonanoic acid	158	C9H18O2	000112-05-0	50
5	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	43





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081663.D
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Sample : G3624-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-SOURCE-6

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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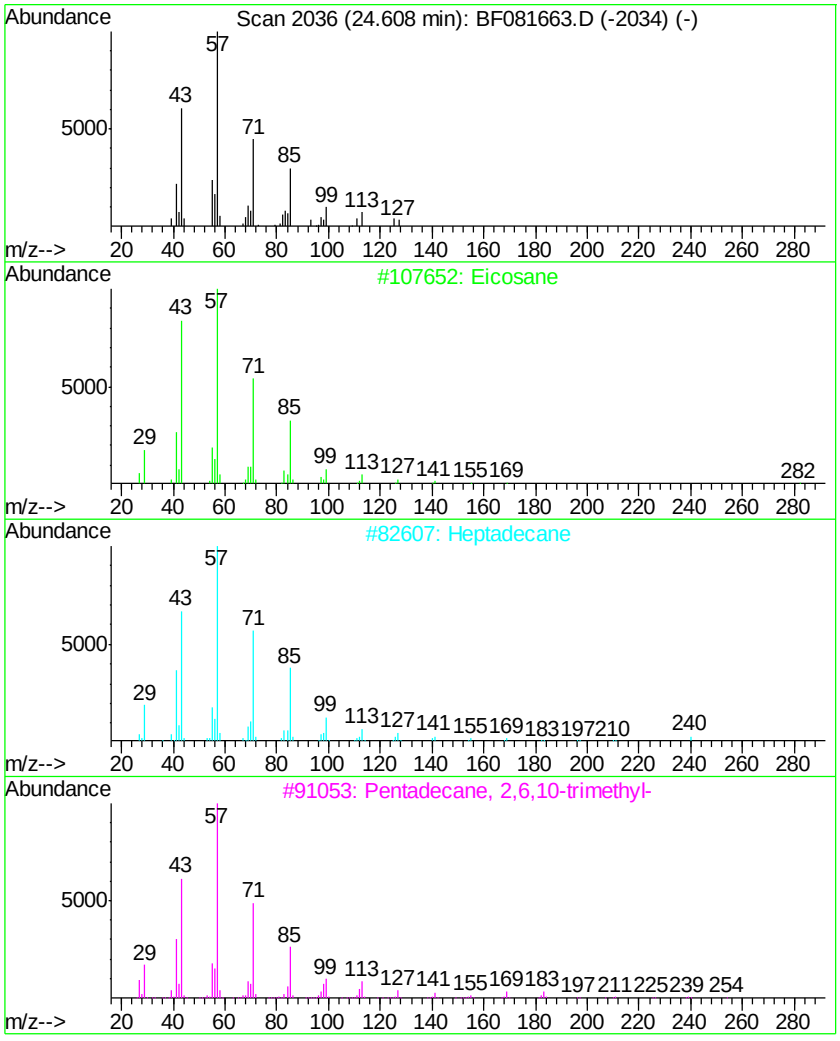
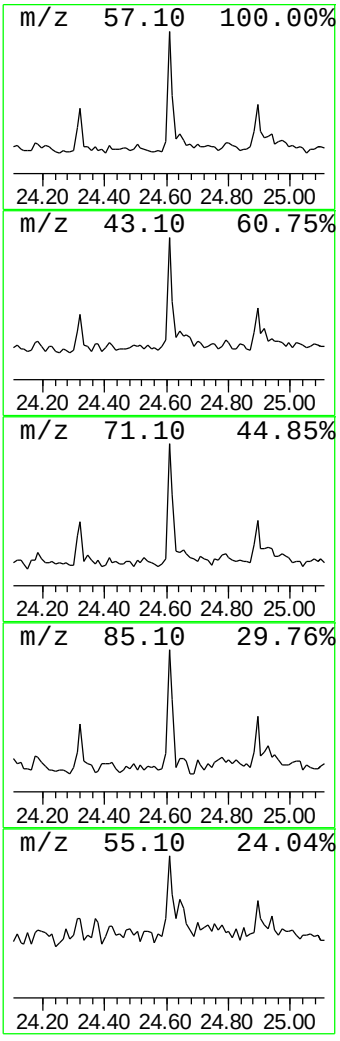
Peak Number 8 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.61	3.32 ng	43682	Perylene-d12	24.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	86
2	Heptadecane	240	C17H36	000629-78-7	86
3	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	78
4	Hexadecane	226	C16H34	000544-76-3	72
5	Pentadecane	212	C15H32	000629-62-9	72





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081663.D
Acq On : 17 Sep 2015 3:01
Operator : UM/IZ
Sample : G3624-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-SOURCE-6

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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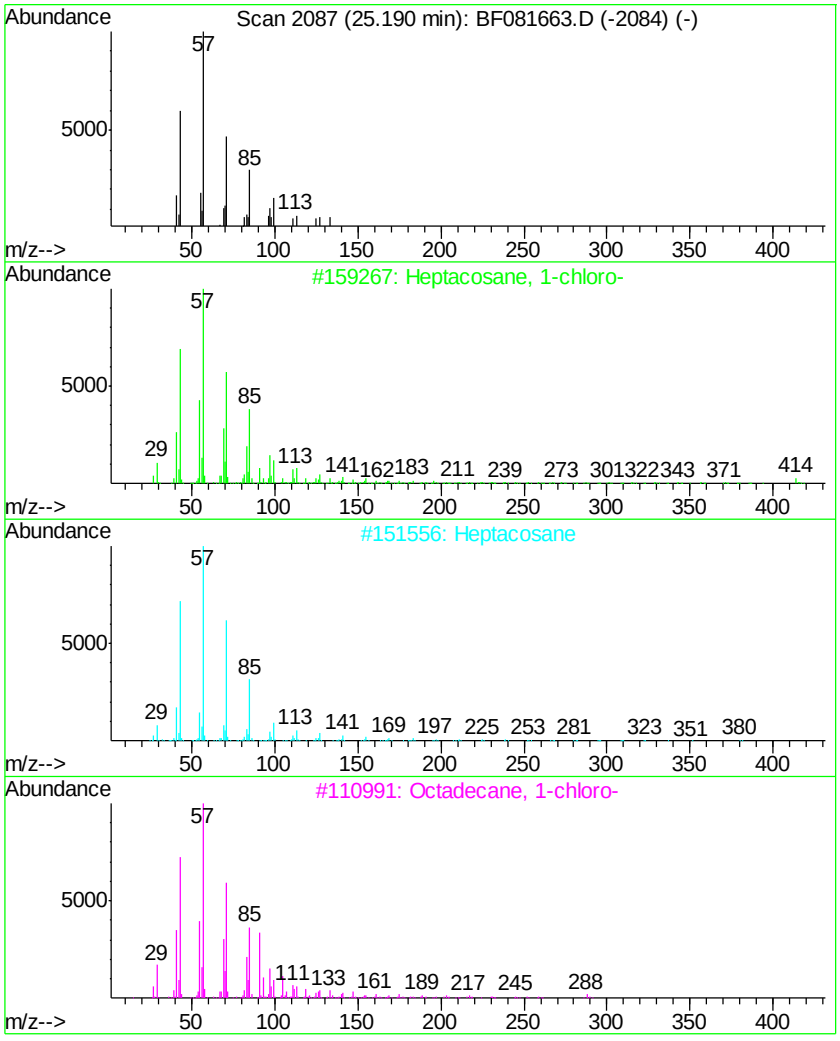
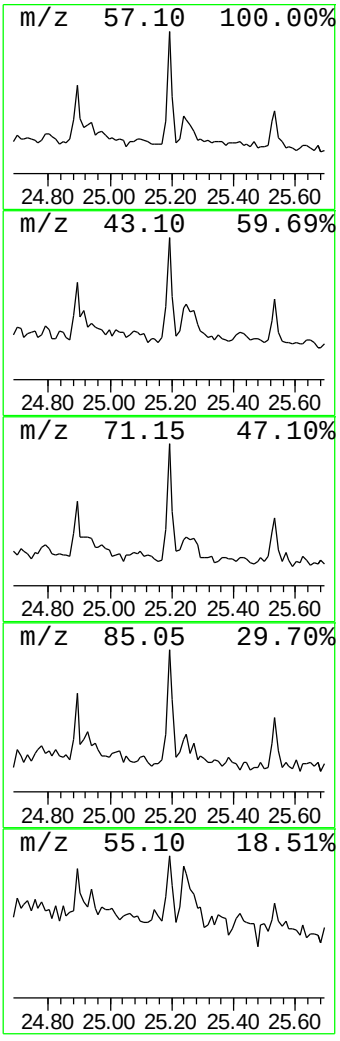
Peak Number 9 Heptacosane, 1-chloro- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.19	2.43 ng	31998	Perylene-d12	24.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	78
2	Heptacosane	380	C27H56	000593-49-7	64
3	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	64
4	Heptadecane	240	C17H36	000629-78-7	64
5	Hexadecane	226	C16H34	000544-76-3	64





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081663.D
Acq On : 17 Sep 2015 3:01
Operator : UM/IZ
Sample : G3624-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-SOURCE-6

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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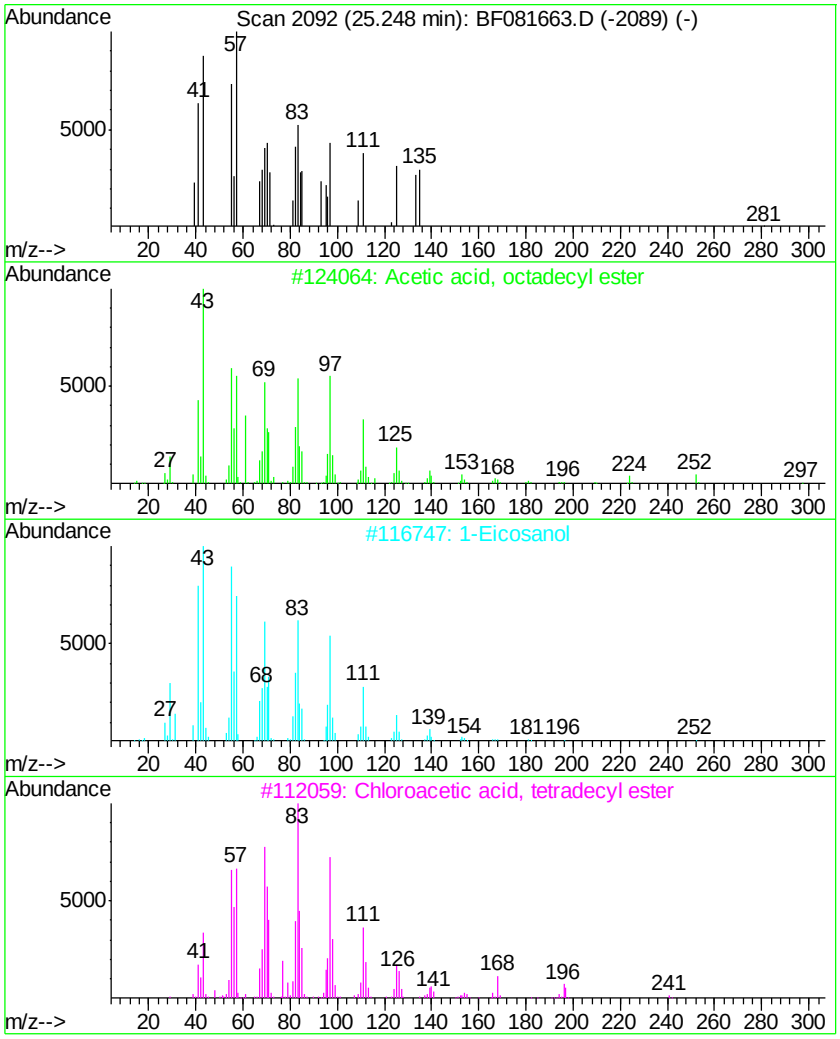
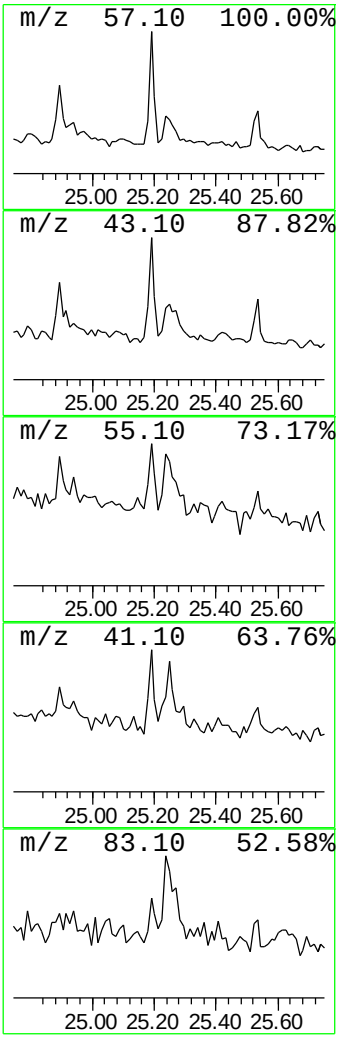
Peak Number 10 unknown25.25 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.25	2.75 ng	36090	Perylene-d12	24.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	47
2	1-Eicosanol	298	C20H42O	000629-96-9	47
3	Chloroacetic acid, tetradecyl ester	290	C16H31ClO2	018277-86-6	46
4	1-Pentadecanol	228	C15H32O	000629-76-5	43
5	3-Octen-2-one, 7-methyl-	140	C9H16O	033046-81-0	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081663.D
Acq On : 17 Sep 2015 3:01
Operator : UM/IZ
Sample : G3624-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-SOURCE-6

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...	4.49	66.1	ng	1079690	1	8.18	326734	20.0
unknown7.70	7.70	114.3	ng	1867390	1	8.18	326734	20.0
Hexadecane	17.75	2.3	ng	53204	4	18.71	466859	20.0
Undecanoic acid	20.47	4.6	ng	107070	4	18.71	466859	20.0
Eicosane	24.61	3.3	ng	43682	6	24.79	262950	20.0
Heptacosane, 1-ch...	25.19	2.4	ng	31998	6	24.79	262950	20.0
unknown25.25	25.25	2.8	ng	36090	6	24.79	262950	20.0