LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088158.D
Acq On : 19 Jun 2016 3:18
Operator : UM/SJ
Sample : H3628-02
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

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-BF060716.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	1.667	6	7	15	rVV	77217	123978	5.53%	0.671%
2	1.781	15	17	39	rVB	895825	1531474	68.35%	8.292%
3	2.810	104	107	114	rVB	18388	35472	1.58%	0.192%
4	4.833	282	284	289	rBV	47881	61495	2.74%	0.333%
5	4.970	293	296	301	rVV	16322	37701	1.68%	0.204%
6	5.096	301	307	314	rVB	13547	37374	1.67%	0.202%
7	5.279	321	323	326	rBV	1043744	1021018	45.57%	5.528%
8	6.193	400	403	414	rBV5	10274	52031	2.32%	0.282%
9	6.341	414	416	424	rBV	657018	755731	33.73%	4.092%
10	6.456	424	426	429	rBV	1830887	1695423	75.67%	9.179%
11	6.536	431	433	440	rVB	21569	48411	2.16%	0.262%
12	6.684	443	446	448	rBV	617023	523711	23.37%	2.835%
13	6.844	457	460	462	rVB	1648239	1841907	82.21%	9.972%
14	7.107	479	483	484	rBV2	12315	23452	1.05%	0.127%
15	7.164	484	488	493	rVV2	55954	135472	6.05%	0.733%
16	7.256	493	496	498	rVV	1357932	1423099	63.52%	7.705%
17	7.359	501	505	507	rVV2	26815	65604	2.93%	0.355%
18	7.450	507	513	516	rVV	83113	205580	9.18%	1.113%
19	7.507	516	518	520	rVV	50727	97072	4.33%	0.526%
20	7.542	520	521	523	rVV	45764	48042	2.14%	0.260%
21	7.576	523	524	528	rVB	20762	34765	1.55%	0.188%
22	7.965	556	558	561	rBV	493319	616934	27.53%	3.340%
23	8.102	566	570	576	rBV2	15699	35202	1.57%	0.191%
24	8.250	581	583	588	rVB4	24387	27962	1.25%	0.151%
25	8.353	588	592	594	rBV4	10032	28489	1.27%	0.154%
26	8.410	594	597	606	rVB6	15773	54686	2.44%	0.296%
27	8.707	621	623	626	rBV	17615	33623	1.50%	0.182%
28	8.787	626	630	636	rVB	14575	46890	2.09%	0.254%
29	9.050	650	653	655	rBV	2452423	2240565	100.00%	12.131%
30	9.176	661	664	666	rVB2	19138	24535	1.10%	0.133%
31	9.450	685	688	689	rVB	25370	26807	1.20%	0.145%
32	9.645	702	705	706	rBV	97835	93902	4.19%	0.508%
33	9.725	709	712	714	rVB	531888	608584	27.16%	3.295%
34	9.896	724	727	730	rBV2	21888	34482	1.54%	0.187%

LSC Area Percent Report

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Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
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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-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.113	743	746	749	rBV3	32220	59065	2.64%	0.320%
36	10.513	778	781	783	rBV	854320	1018260	45.45%	5.513%
37	10.570	785	786	790	rVB	20080	33003	1.47%	0.179%
38	10.628	790	791	795	rBV	65685	74736	3.34%	0.405%
39	11.096	829	832	834	rVB2	50551	59121	2.64%	0.320%
40	11.199	838	841	843	rBV	620992	520491	23.23%	2.818%
41	11.748	887	889	892	rBV2	25150	46056	2.06%	0.249%
42	11.931	904	905	910	rVB5	37651	47716	2.13%	0.258%
43	12.616	963	965	967	rVB	19266	25349	1.13%	0.137%
44	12.674	968	970	974	rVB	18029	35825	1.60%	0.194%
45	12.788	977	980	982	rBV	1516993	1863995	83.19%	10.092%
46	13.348	1027	1029	1032	rBV2	34984	55285	2.47%	0.299%
47	13.714	1058	1061	1067	rVB2	31777	52694	2.35%	0.285%
48	13.828	1069	1071	1074	rBV	556799	496761	22.17%	2.690%
49	14.331	1113	1115	1117	rVB3	19212	26034	1.16%	0.141%
50	15.211	1189	1192	1199	rVB	311230	384095	17.14%	2.080%

Sum of corrected areas: 18469959

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088158.D
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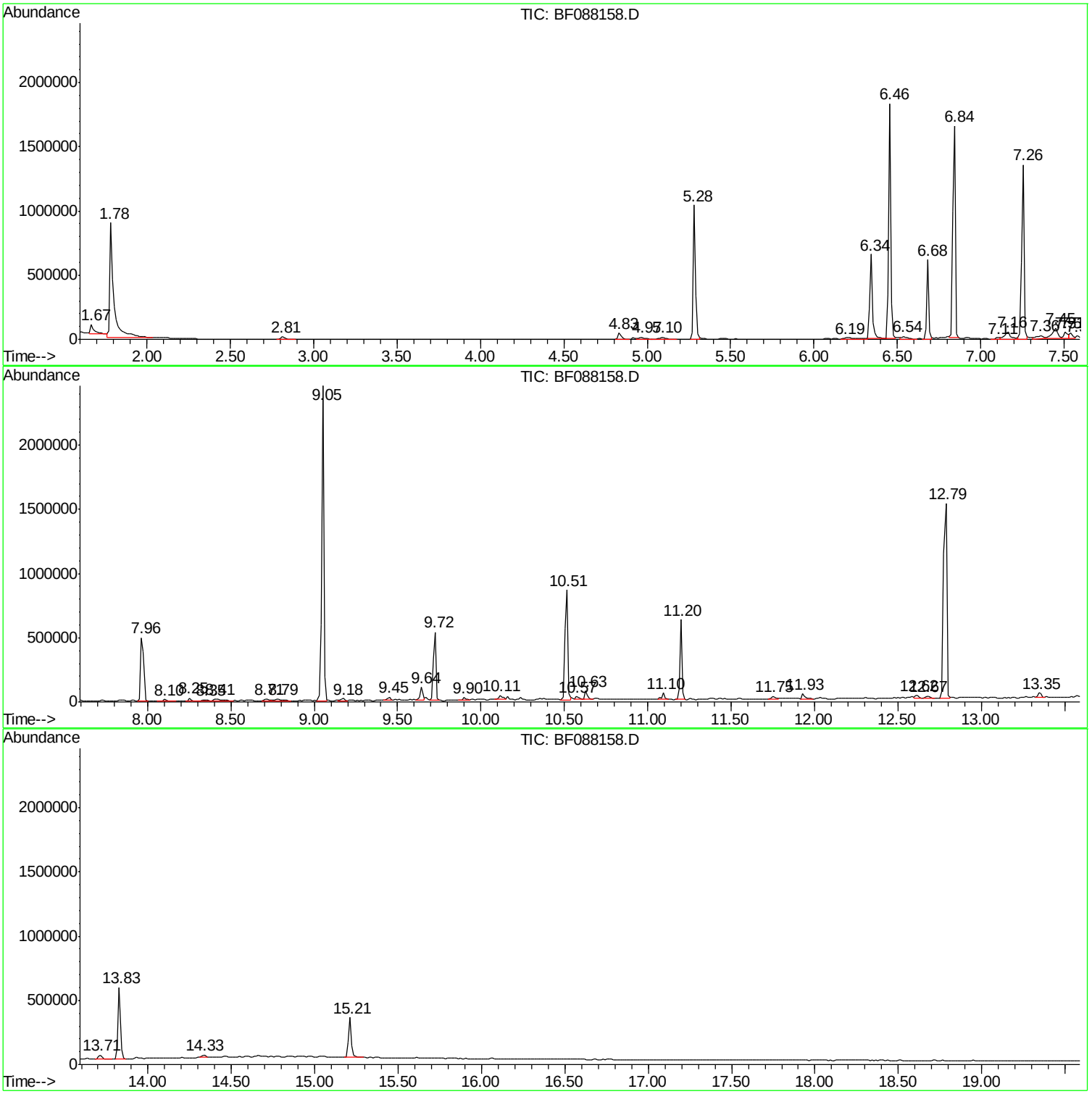
Operator : UM/SJ
Sample : H3628-02
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088158.D
Acq On : 19 Jun 2016 3:18
Operator : UM/SJ
Sample : H3628-02
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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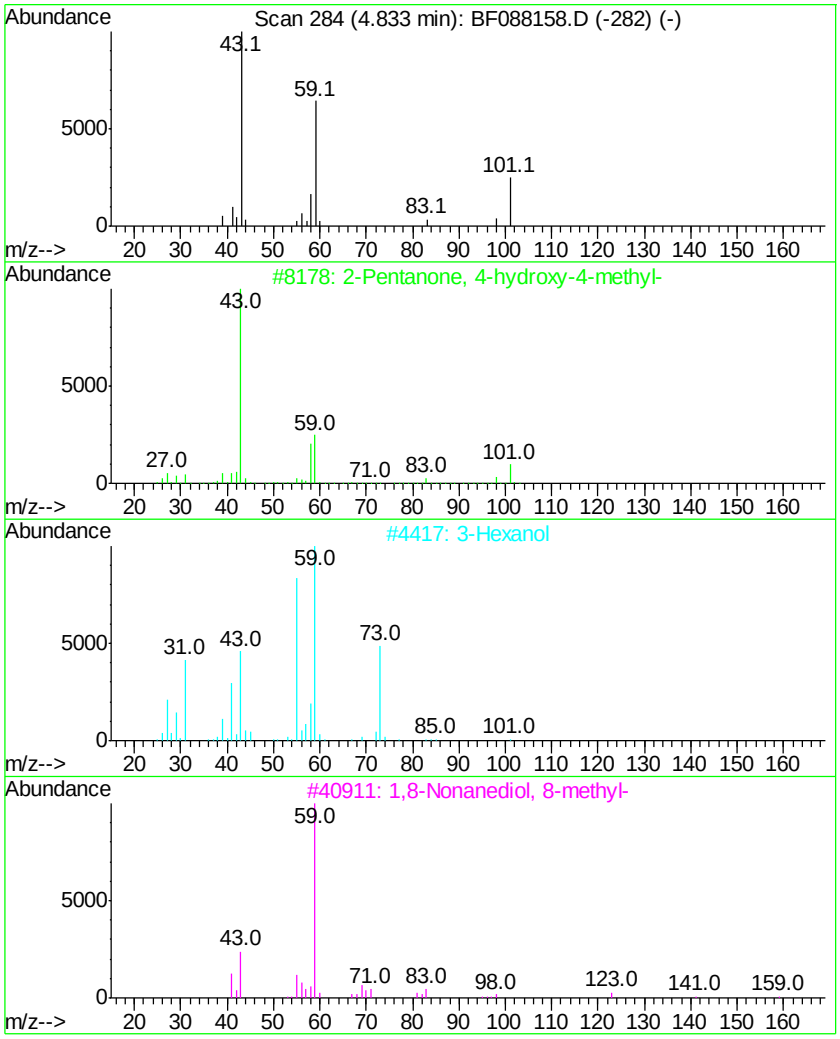
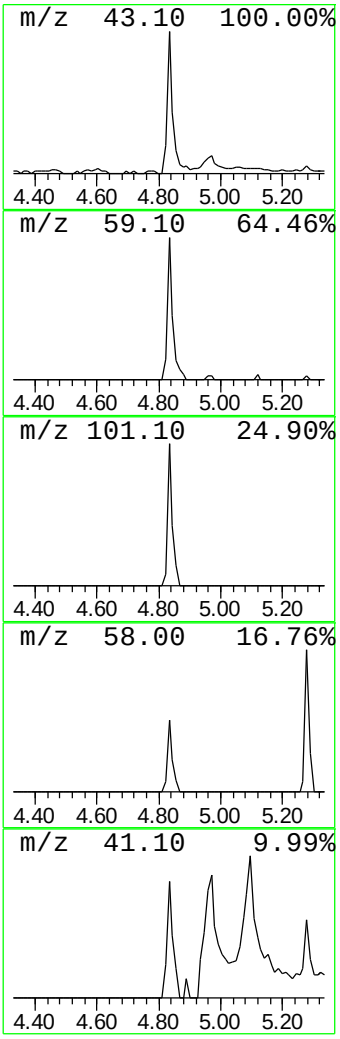
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	2.35 ng	61495	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol	102	C6H14O	000623-37-0	28
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088158.D
Acq On : 19 Jun 2016 3:18
Operator : UM/SJ
Sample : H3628-02
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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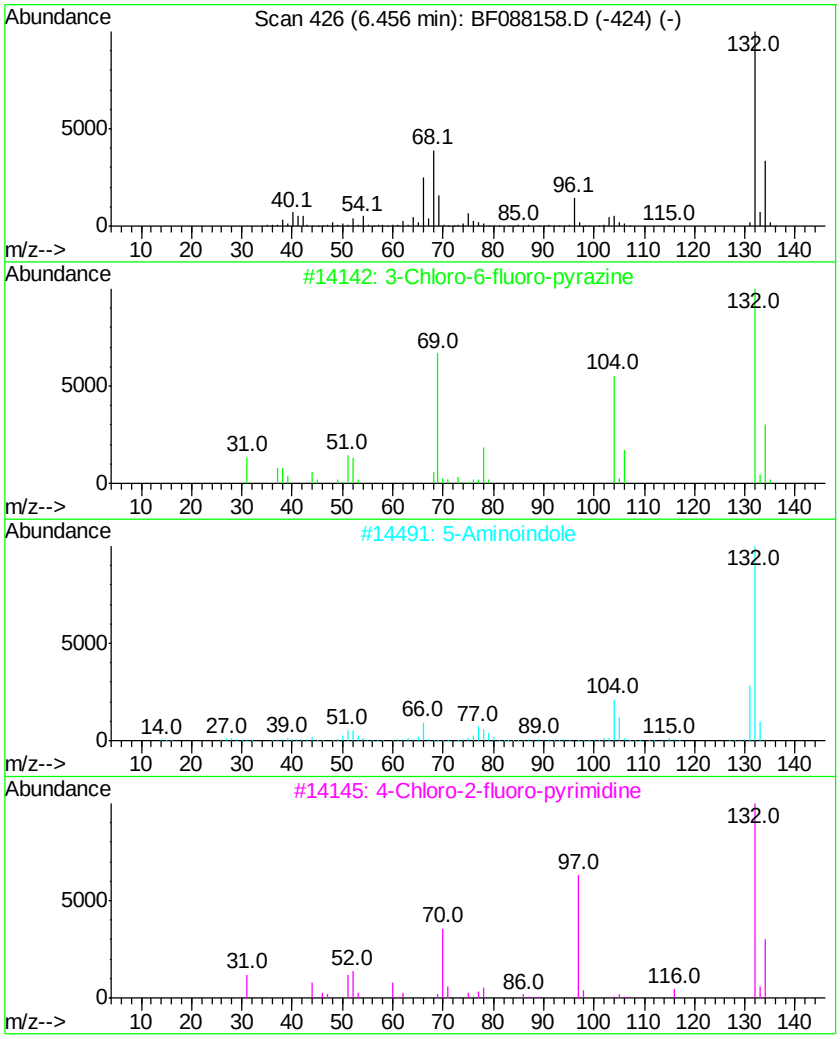
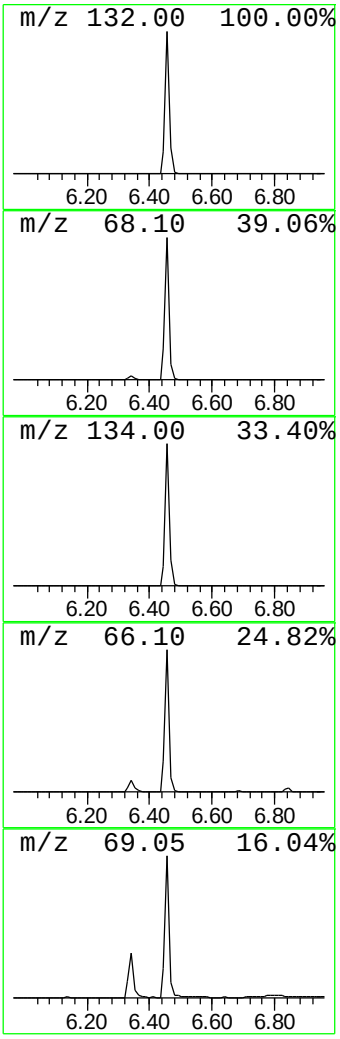
Peak Number 4 unknown6.46 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	64.75 ng	1695420	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088158.D
Acq On : 19 Jun 2016 3:18
Operator : UM/SJ
Sample : H3628-02
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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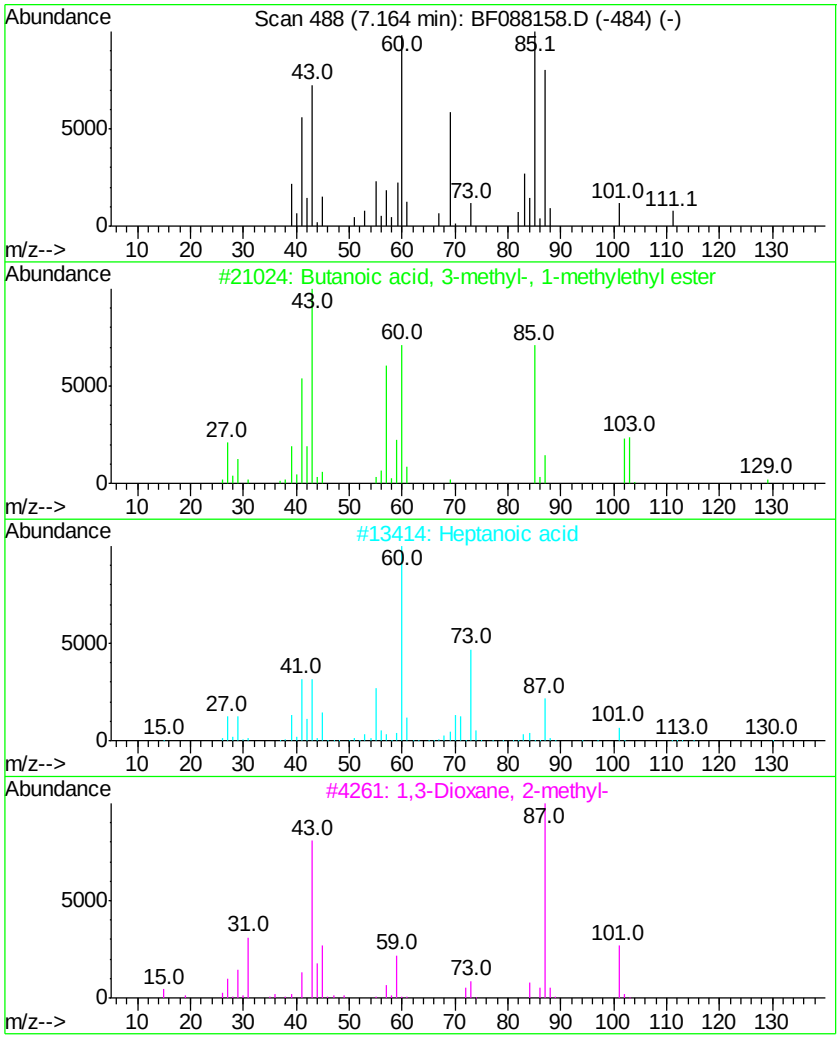
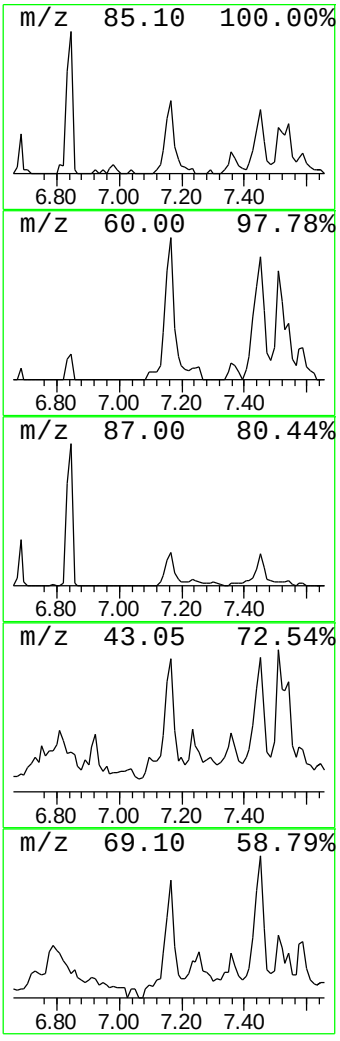
Peak Number 6 unknown7.16 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.16	5.17 ng	135472	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-, 1-meth...	144	C8H16O2	032665-23-9	35
2	Heptanoic acid	130	C7H14O2	000111-14-8	25
3	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	22
4	Ethanol, 2-(2-butoxyethoxy)-, ac...	204	C10H20O4	000124-17-4	16
5	1-Pentanol, 2,2-dimethyl-	116	C7H16O	002370-12-9	14





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088158.D
Acq On : 19 Jun 2016 3:18
Operator : UM/SJ
Sample : H3628-02
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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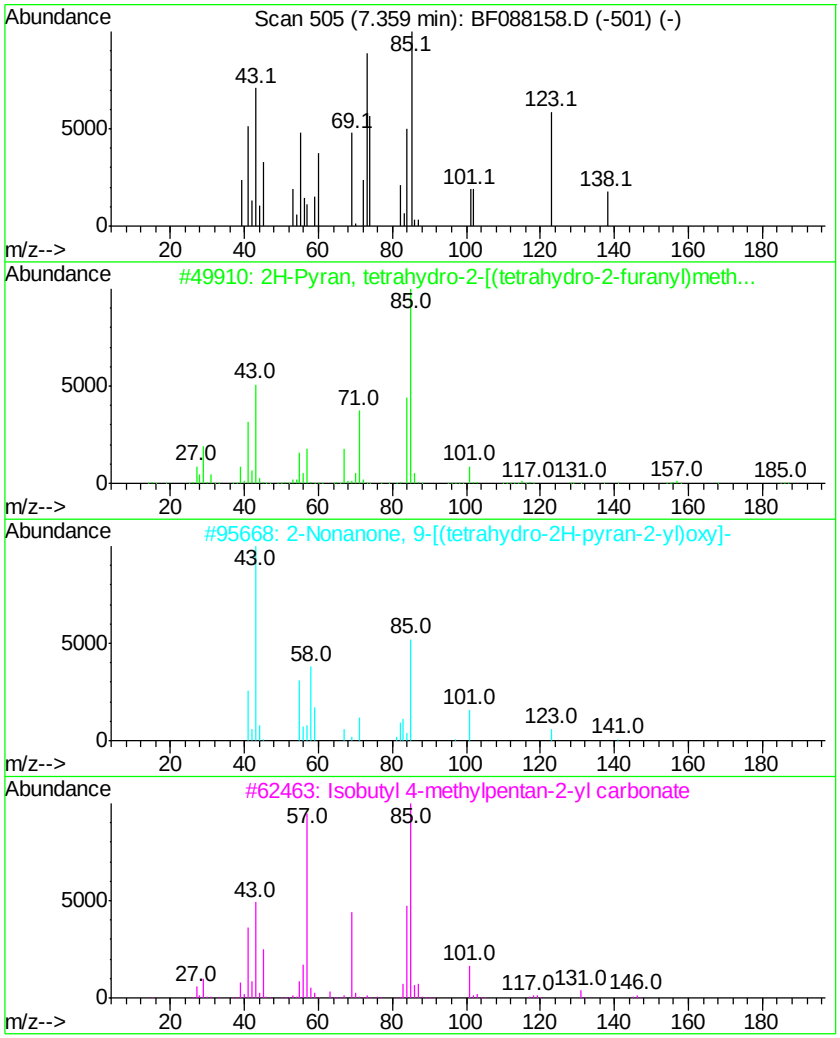
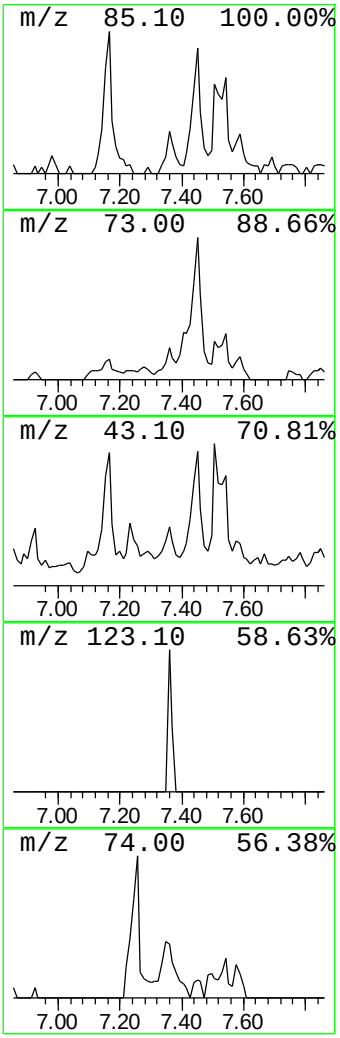
Peak Number 7 unknown7.36 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.36	2.13 ng	65604	Naphthalene-d8	7.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Pyran, tetrahydro-2-[(tetrahy...	186	C10H18O3	000710-14-5	35
2	2-Nonanone, 9-[(tetrahydro-2H-py...	242	C14H26O3	054699-41-1	27
3	Isobutyl 4-methylpentan-2-yl car...	202	C11H22O3	1000372-76-2	25
4	1-Hexanol, 6-[(tetrahydro-2H-pyr...	202	C11H22O3	028659-22-5	14
5	3-Methylpentan-3-yl propyl carbo...	188	C10H20O3	1000372-82-3	12





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Instrument : BNA_F
ClientSampleId : W-27

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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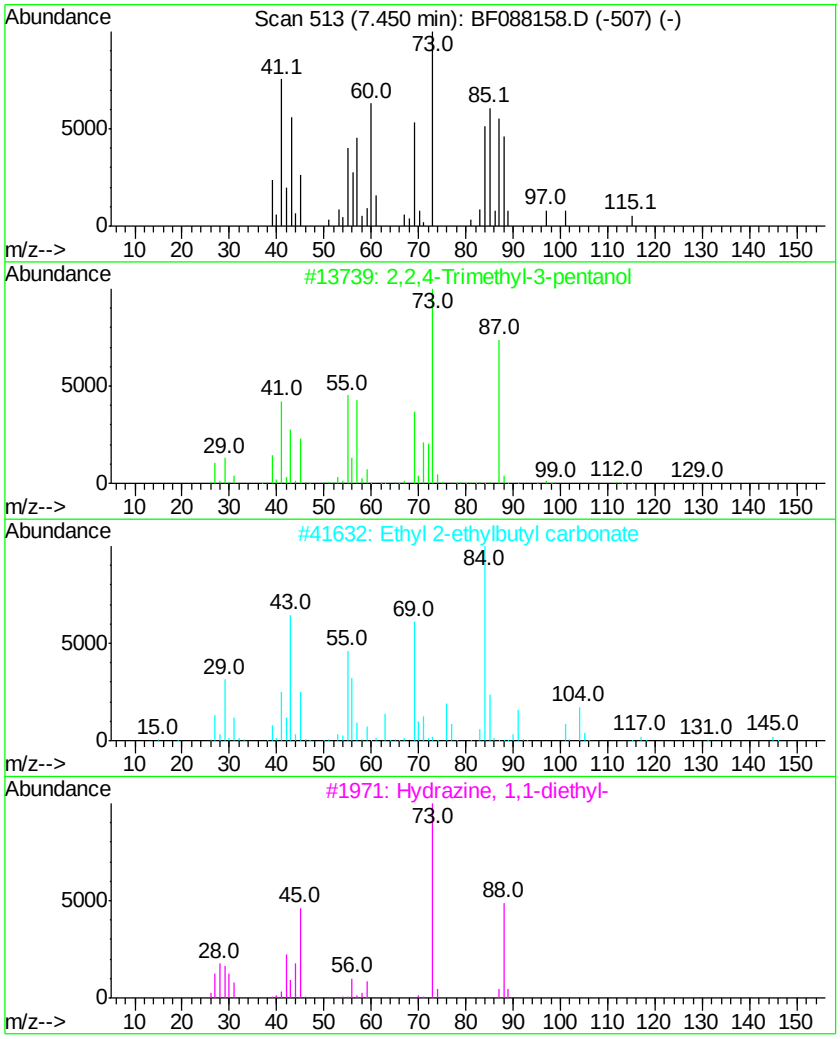
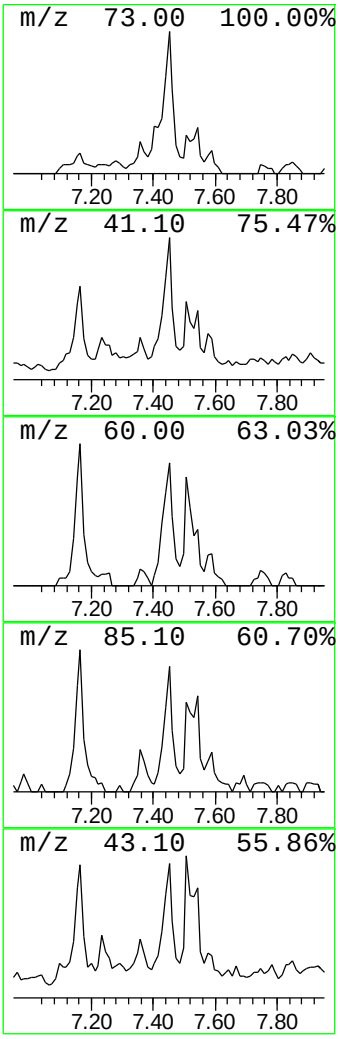
Peak Number 8 unknown7.45 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.45	6.66 ng	205580	Naphthalene-d8	7.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	22
2	Ethyl 2-ethylbutyl carbonate	174	C9H18O3	1000373-79-7	22
3	Hydrazine, 1,1-diethyl-	88	C4H12N2	000616-40-0	22
4	3-Ethyl-3-methyl-2-pentanol	130	C8H18O	066576-22-5	16
5	3-Pentanol, 2,3-dimethyl-	116	C7H16O	000595-41-5	14





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Data File : BF088158.D
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Sample : H3628-02
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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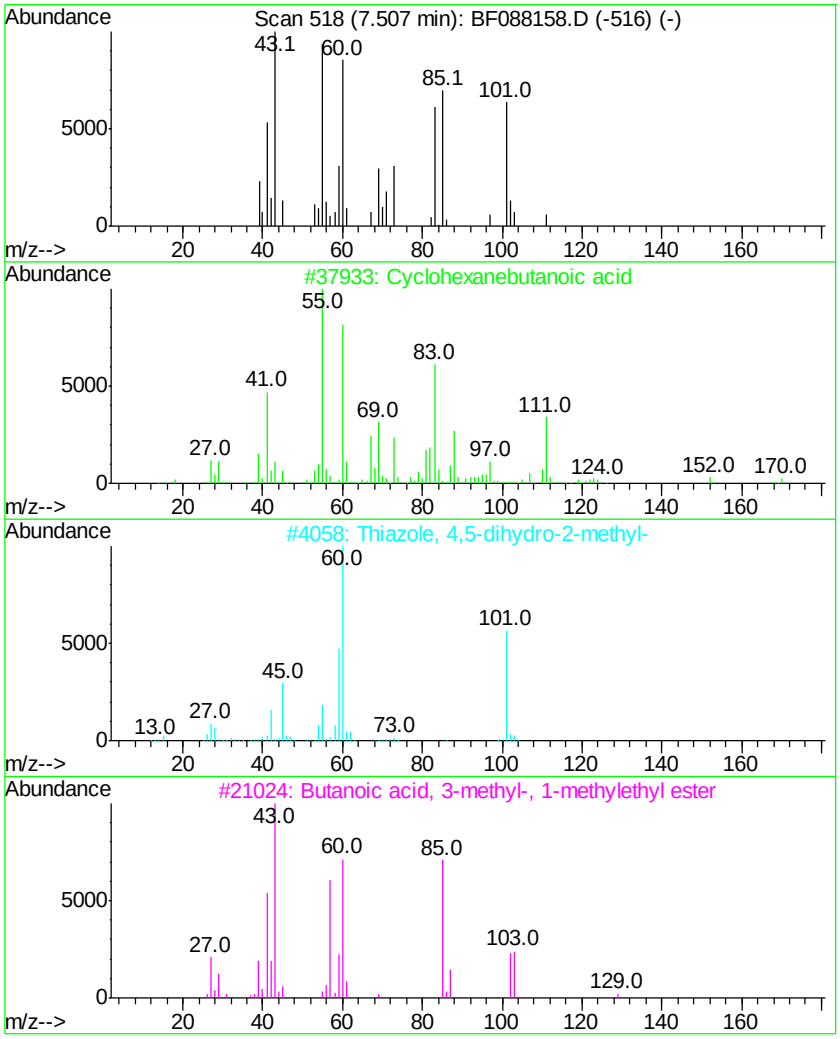
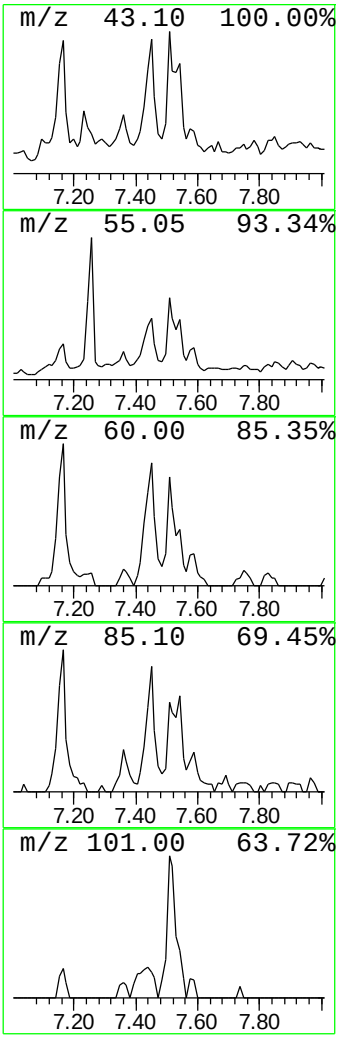
Peak Number 9 unknown7.51 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.51	3.15 ng	97072	Naphthalene-d8	7.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanebutanoic acid	170	C10H18O2	004441-63-8	43
2	Thiazole, 4,5-dihydro-2-methyl-	101	C4H7NS	002346-00-1	38
3	Butanoic acid, 3-methyl-, 1-meth...	144	C8H16O2	032665-23-9	32
4	Cyclobutanecarboxylic acid, prop...	142	C8H14O2	1000280-40-0	25
5	3-Methyl-2-butenoic acid, hexade...	324	C21H40O2	060129-26-2	22





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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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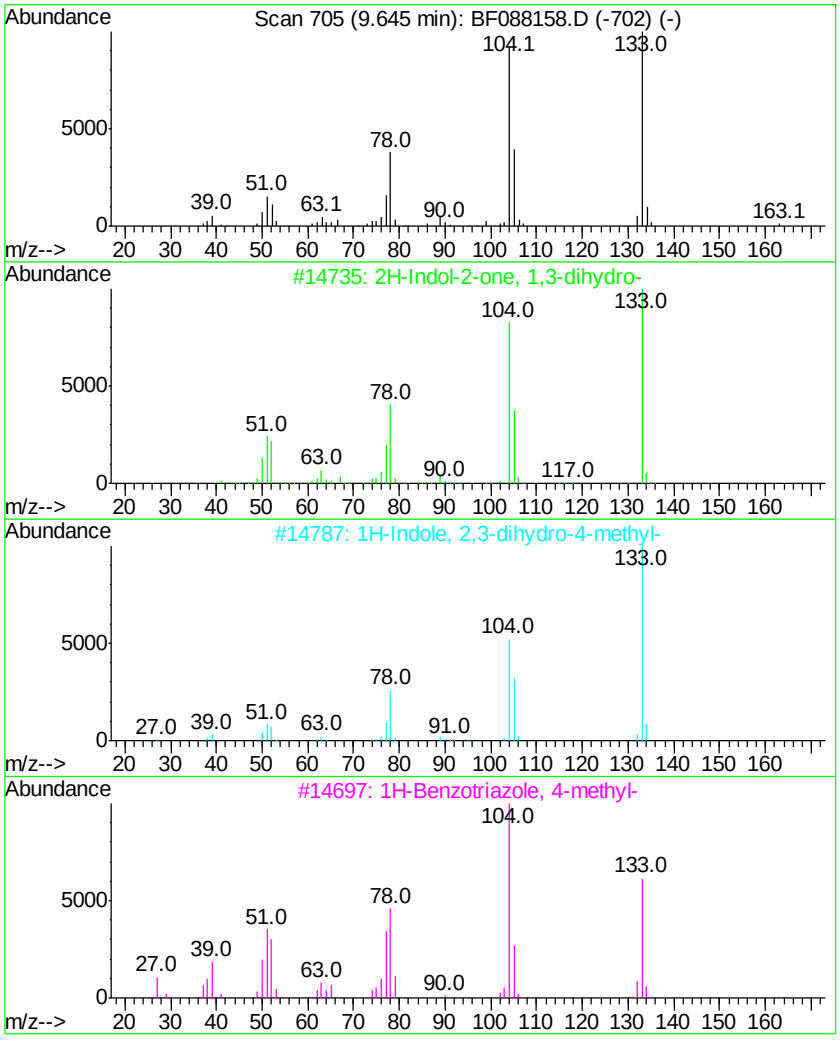
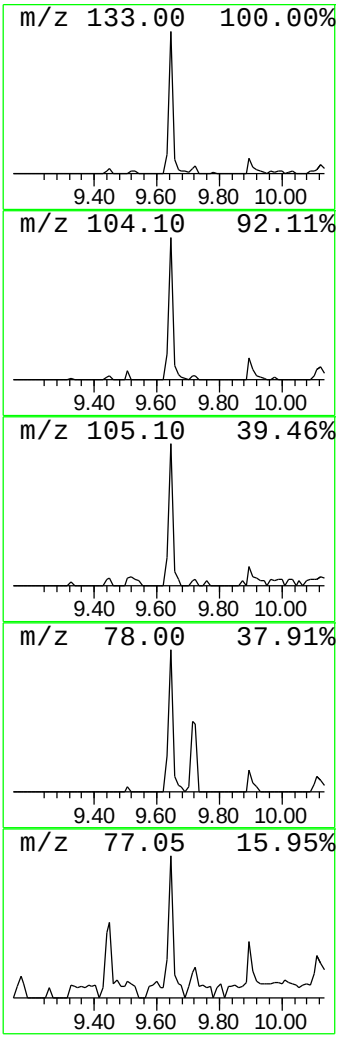
Peak Number 10 2H-Indol-2-one, 1,3-dihydro- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.64	3.09 ng	93902	Acenaphthene-d10	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Indol-2-one, 1,3-dihydro-	133	C8H7NO	000059-48-3	95
2	1H-Indole, 2,3-dihydro-4-methyl-	133	C9H11N	062108-16-1	91
3	1H-Benzotriazole, 4-methyl-	133	C7H7N3	029878-31-7	90
4	1H-Benzotriazole, 5-methyl-	133	C7H7N3	000136-85-6	87
5	Benzene, 1-isocyanato-3-methyl-	133	C8H7NO	000621-29-4	83





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088158.D
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Operator : UM/SJ
Sample : H3628-02
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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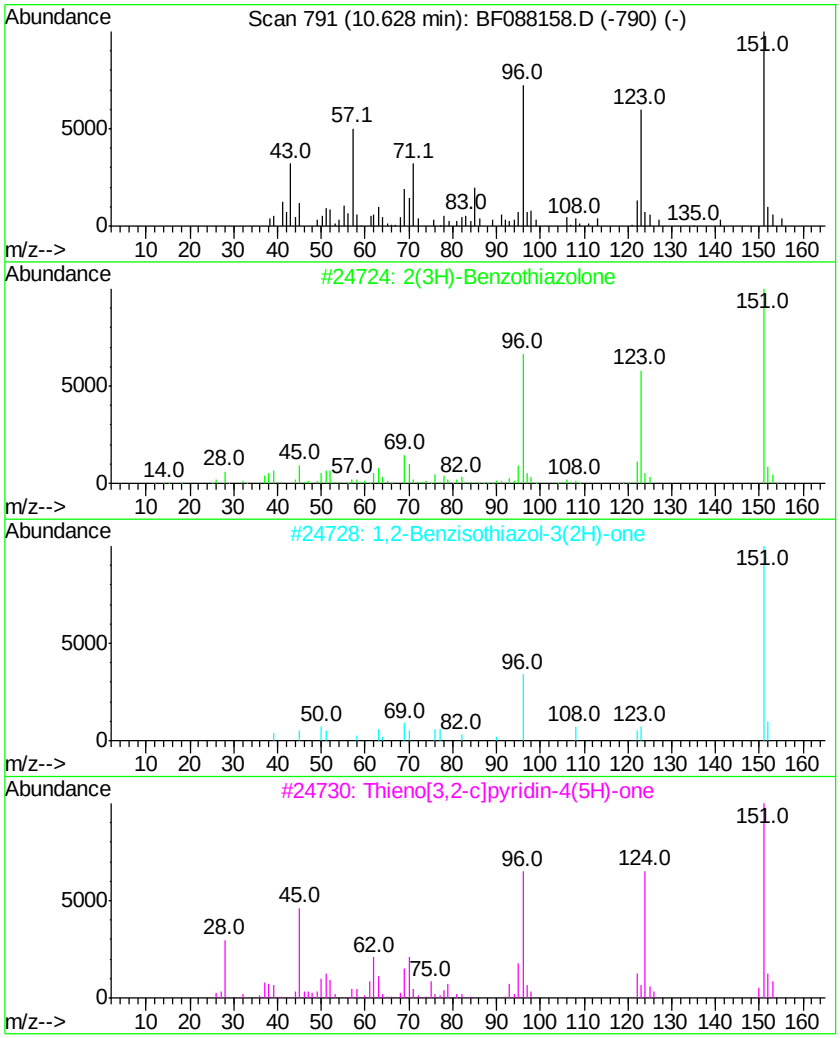
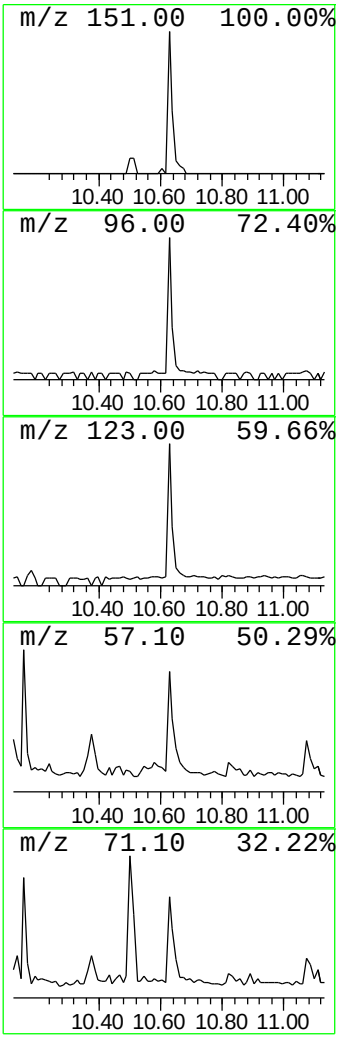
Peak Number 11 2(3H)-Benzothiazolone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	2.87 ng	74736	Phenanthrene-d10	11.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	93
2	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	53
3	Thieno[3,2-c]pyridin-4(5H)-one	151	C7H5NOS	027685-92-3	52
4	Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	47
5	Benzooxazole-2-thiol	151	C7H5NOS	1000318-31-6	38





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Data File : BF088158.D
Acq On : 19 Jun 2016 3:18
Operator : UM/SJ
Sample : H3628-02
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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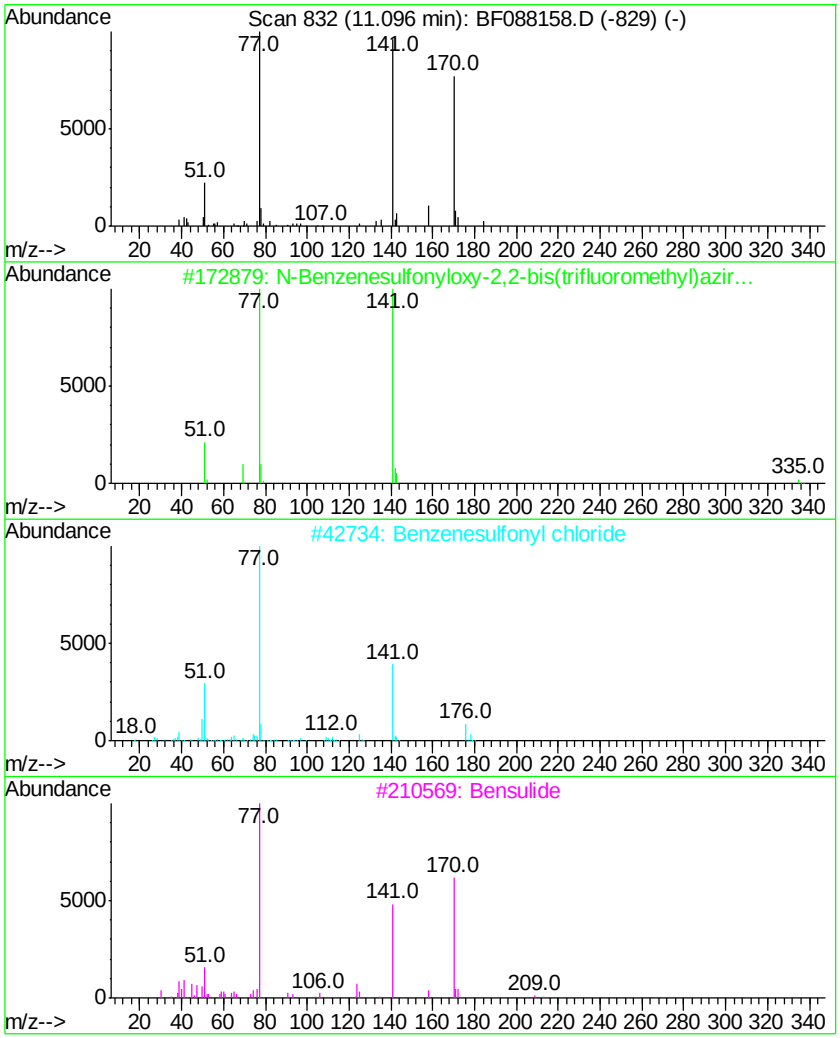
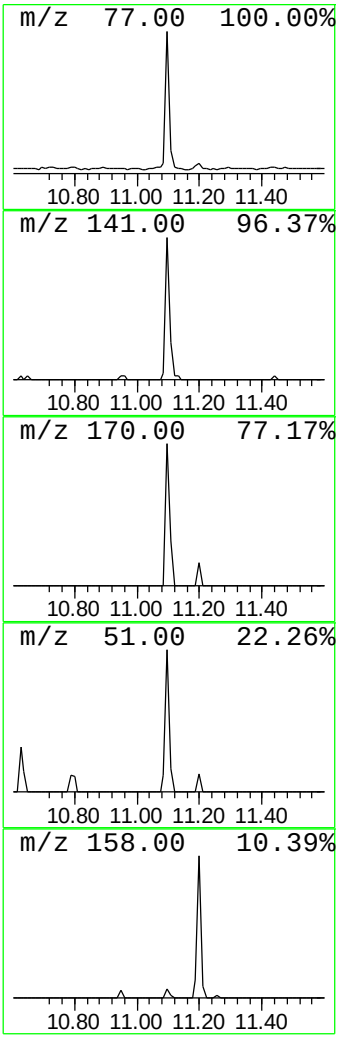
Peak Number 12 unknown11.10 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.10	2.27 ng	59121	Phenanthrene-d10	11.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-Benzenesulfonyloxy-2,2-bis(tri...	335	C10H7F6NO3S	055734-41-3	40
2	Benzenesulfonyl chloride	176	C6H5ClO2S	000098-09-9	38
3	Bensulide	397	C14H24NO4PS3	000741-58-2	38
4	1H,3H-Naphtho[1,8-cd]pyran	170	C12H10O	000203-84-9	37
5	N,N-Dichlorobenzenesulfonamide	225	C6H5Cl2NO2S	000473-29-0	35





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Data File : BF088158.D
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Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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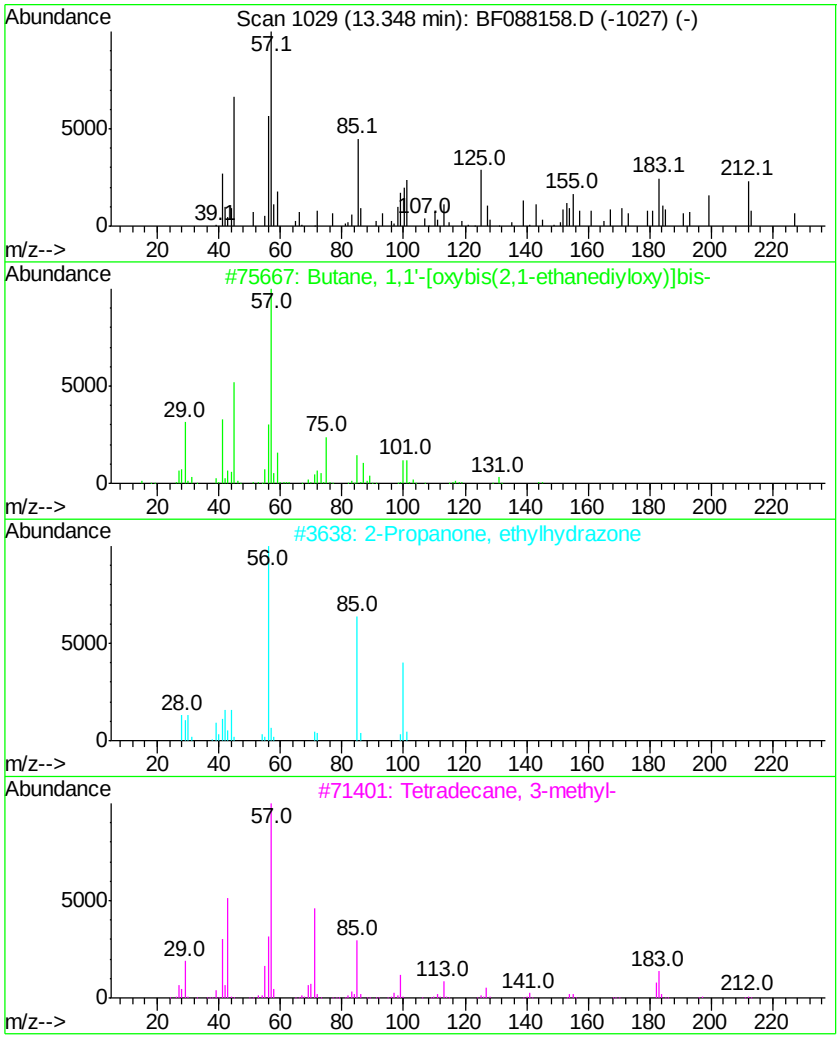
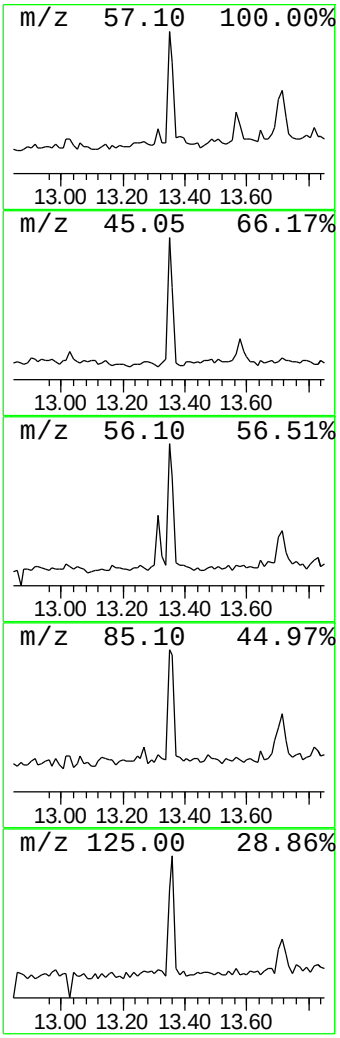
Peak Number 13 unknown13.35 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	2.23 ng	55285	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	35
2	2-Propanone, ethylhydrazone	100	C5H12N2	007422-99-3	27
3	Tetradecane, 3-methyl-	212	C15H32	018435-22-8	25
4	Dodecane, 3-methyl-	184	C13H28	017312-57-1	14
5	Decane, 2,5,6-trimethyl-	184	C13H28	062108-23-0	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088158.D
Acq On : 19 Jun 2016 3:18
Operator : UM/SJ
Sample : H3628-02
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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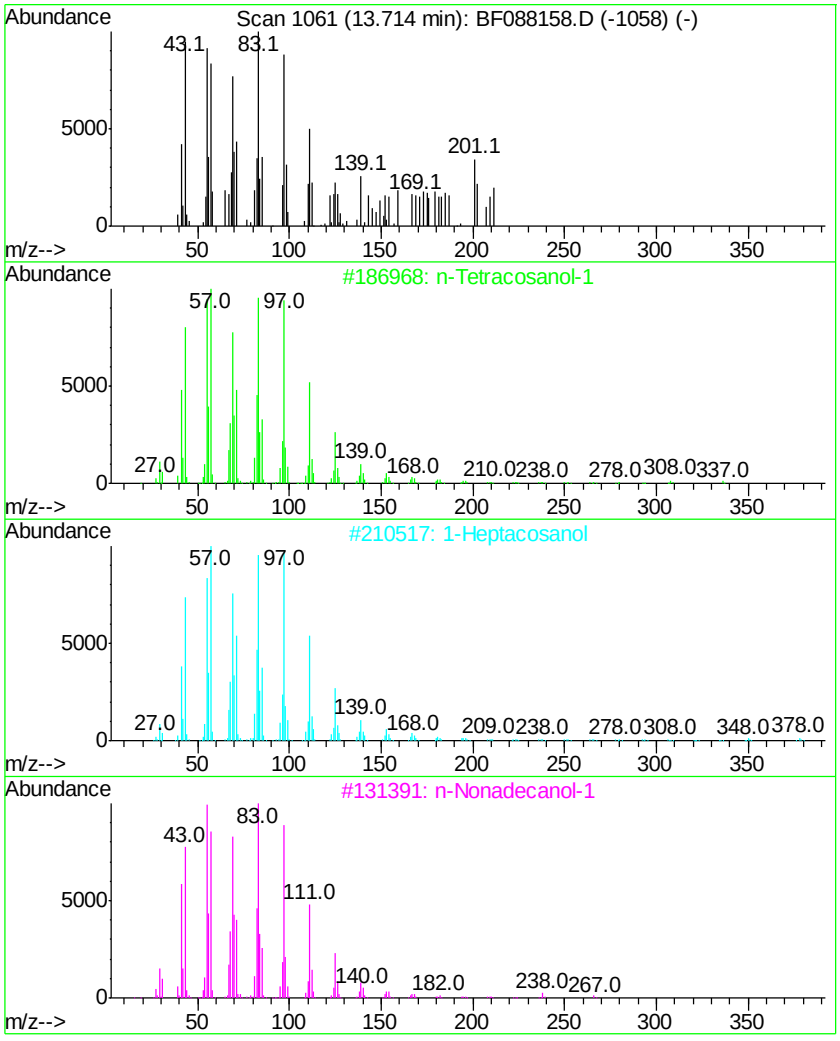
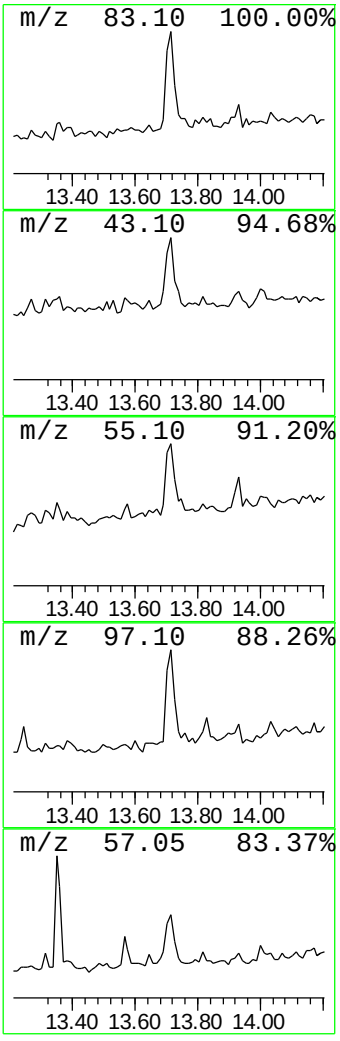
Peak Number 14 n-Tetracosanol-1 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	2.12 ng	52694	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	76
2	1-Heptacosanol	396	C27H56O	002004-39-9	76
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	76
4	Behenic alcohol	326	C22H46O	000661-19-8	76
5	1-Heneicosanol	312	C21H44O	015594-90-8	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061816\
Data File : BF088158.D
Acq On : 19 Jun 2016 3:18
Operator : UM/SJ
Sample : H3628-02
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.83	2.4	ng	61495	1	6.68	523711	20.0
unknown6.46	6.46	64.8	ng	1695420	1	6.68	523711	20.0
unknown7.16	7.16	5.2	ng	135472	1	6.68	523711	20.0
unknown7.36	7.36	2.1	ng	65604	2	7.96	616934	20.0
unknown7.45	7.45	6.7	ng	205580	2	7.96	616934	20.0
unknown7.51	7.51	3.1	ng	97072	2	7.96	616934	20.0
2H-Indol-2-one, 1...	9.64	3.1	ng	93902	3	9.72	608584	20.0
2(3H)-Benzothiazo...	10.63	2.9	ng	74736	4	11.20	520491	20.0
unknown11.10	11.10	2.3	ng	59121	4	11.20	520491	20.0
unknown13.35	13.35	2.2	ng	55285	5	13.83	496761	20.0
n-Tetracosanol-1	13.71	2.1	ng	52694	5	13.83	496761	20.0