LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052816\
Data File : BF087488.D
Acq On : 28 May 2016 20:01
Operator : UM/SJ
Sample : H3276-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-01

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-BF052316.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	4.684	269	271	295	rBV	198497	609706	14.62%	1.837%
2	5.359	328	330	361	rBV	797019	1904687	45.67%	5.739%
3	5.953	380	382	393	rBV	42866	101429	2.43%	0.306%
4	7.016	472	475	482	rBV	614200	1135739	27.23%	3.422%
5	7.119	482	484	505	rVB	2158786	3253977	78.02%	9.804%
6	7.462	512	514	523	rBV	536014	808409	19.38%	2.436%
7	7.702	532	535	551	rVV	1913994	2983752	71.54%	8.990%
8	7.907	551	553	560	rVB2	23699	56215	1.35%	0.169%
9	8.342	586	591	592	rBV2	61514	128095	3.07%	0.386%
10	8.376	592	594	607	rVB	1449166	2415241	57.91%	7.277%
11	8.719	622	624	626	rBV	69538	89558	2.15%	0.270%
12	8.765	626	628	631	rVB	33152	48607	1.17%	0.146%
13	9.005	647	649	654	rVB2	40824	64862	1.56%	0.195%
14	9.096	654	657	663	rVB2	114047	196629	4.71%	0.592%
15	9.496	689	692	698	rBV	781737	1151479	27.61%	3.469%
16	9.599	698	701	708	rVB2	63350	137875	3.31%	0.415%
17	9.976	731	734	737	rBV2	37461	51825	1.24%	0.156%
18	10.148	747	749	753	rVB	41927	65499	1.57%	0.197%
19	10.273	757	760	763	rVV	90198	142250	3.41%	0.429%
20	10.342	763	766	770	rVV3	22573	54165	1.30%	0.163%
21	10.433	770	774	776	rVV2	25638	59344	1.42%	0.179%
22	10.468	776	777	780	rVV	46823	53863	1.29%	0.162%
23	10.582	782	787	790	rVV2	80694	139890	3.35%	0.421%
24	10.811	803	807	810	rBV	502598	743973	17.84%	2.242%
25	11.279	844	848	850	rBV	3115991	4170826	100.00%	12.567%
26	11.496	863	867	870	rBV2	30190	71467	1.71%	0.215%
27	11.588	874	875	880	rVB2	38382	62687	1.50%	0.189%
28	11.691	880	884	887	rBV2	35670	90555	2.17%	0.273%
29	11.805	891	894	896	rVV	139912	213894	5.13%	0.644%
30	11.851	896	898	904	rVV2	55999	111238	2.67%	0.335%
31	11.976	906	909	916	rVV2	101786	275845	6.61%	0.831%
32	12.114	918	921	924	rBV	116779	150545	3.61%	0.454%
33	12.319	936	939	943	rBV	860818	1182060	28.34%	3.562%
34	12.376	943	944	947	rVV2	41801	78653	1.89%	0.237%

LSC Area Percent Report

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Operator : UM/SJ
Sample : H3276-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-01

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-BF052316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.434	947	949	955	rVB6	17767	52244	1.25%	0.157%
36	12.548	955	959	961	rBV	21247	42867	1.03%	0.129%
37	12.696	966	972	974	rBV3	48946	113130	2.71%	0.341%
38	12.765	974	978	980	rVB2	31994	56859	1.36%	0.171%
39	12.868	984	987	990	rBV	51042	91971	2.21%	0.277%
40	12.925	990	992	994	rBV	39617	47102	1.13%	0.142%
41	13.005	997	999	1001	rBV2	22733	47159	1.13%	0.142%
42	13.165	1007	1013	1015	rBV2	48692	81063	1.94%	0.244%
43	13.222	1016	1018	1023	rVB	56397	87117	2.09%	0.262%
44	13.314	1023	1026	1029	rBV	61105	108220	2.59%	0.326%
45	13.508	1040	1043	1046	rBV3	23783	52405	1.26%	0.158%
46	13.622	1050	1053	1063	rBV	1604800	2646033	63.44%	7.972%
47	13.931	1077	1080	1082	rBV	44684	71807	1.72%	0.216%
48	14.720	1147	1149	1158	rBV	766064	1153801	27.66%	3.476%
49	14.937	1166	1168	1171	rBV2	27102	45493	1.09%	0.137%
50	15.714	1232	1236	1244	rBV3	57792	119436	2.86%	0.360%
51	16.823	1330	1333	1336	rBV	22444	45244	1.08%	0.136%
52	17.085	1353	1356	1358	rBV	3324389	3968376	95.15%	11.957%
53	18.434	1471	1474	1486	rBV	583972	939503	22.53%	2.831%
54	20.103	1618	1620	1630	rBV	412432	615166	14.75%	1.853%

Sum of corrected areas: 33189835

LSC Report - Integrated Chromatogram

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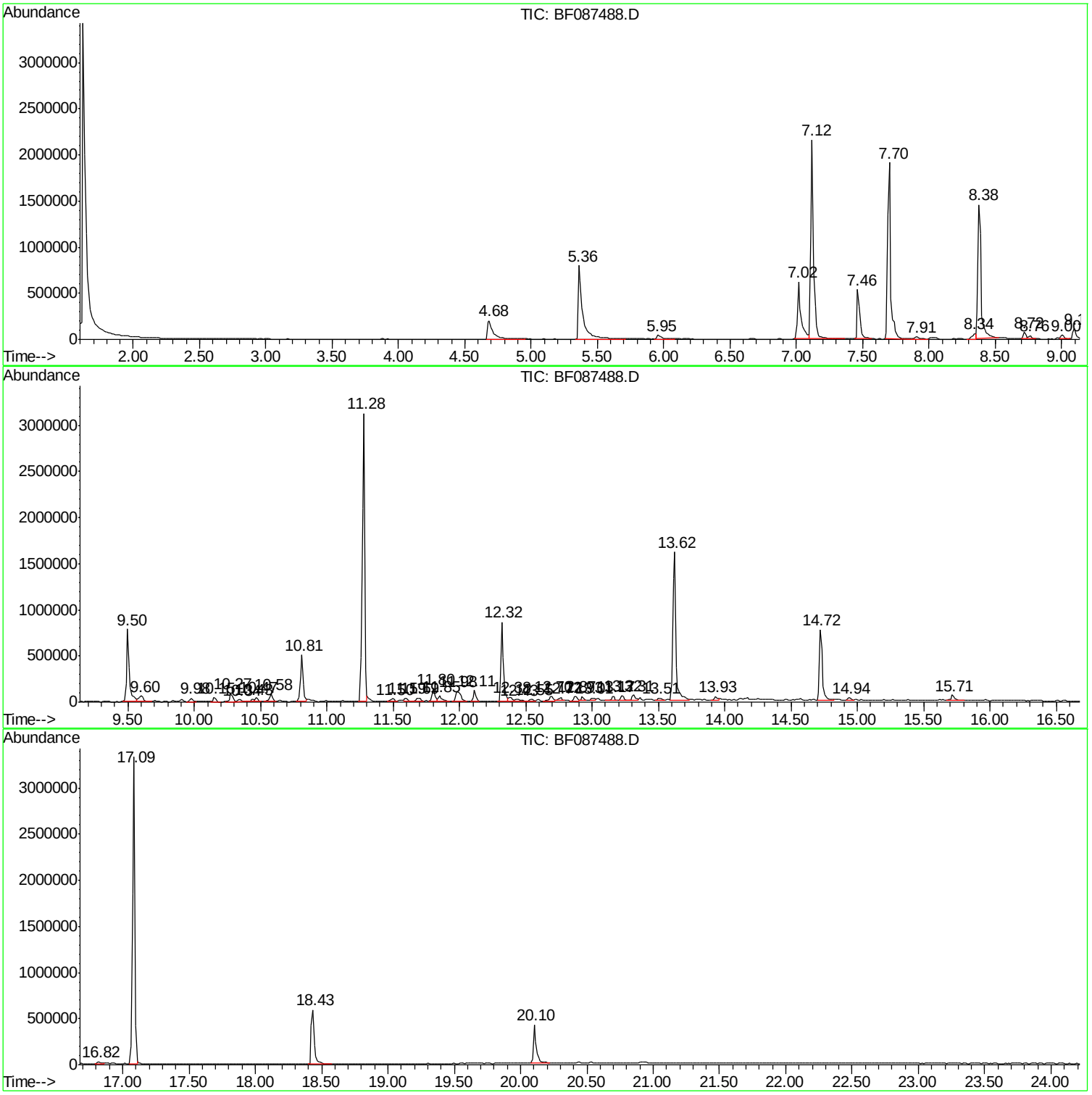
Data File : BF087488.D
Acq On : 28 May 2016 20:01
Operator : UM/SJ
Sample : H3276-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052816\
Data File : BF087488.D
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ALS Vial : 15 Sample Multiplier: 1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

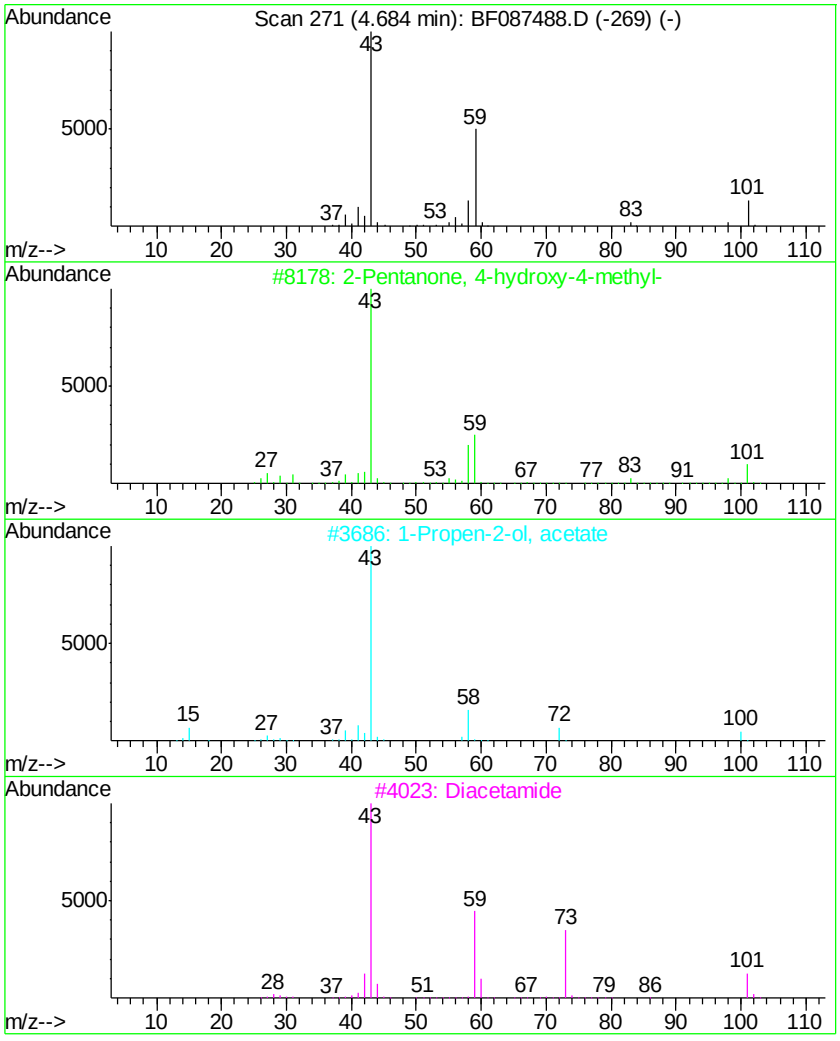
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

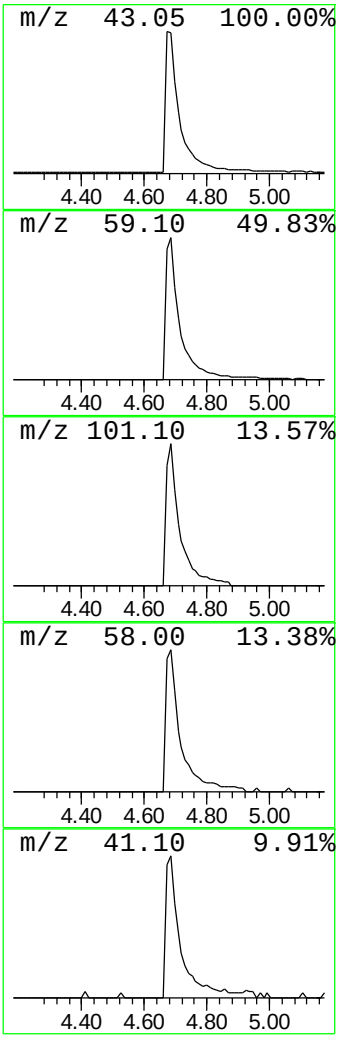
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.68	15.08 ng	609706	1,4-Dichlorobenzene-d4	7.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3	Diacetamide	101	C4H7NO2	000625-77-4	9
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5	Butane	58	C4H10	000106-97-8	9





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Sample : H3276-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

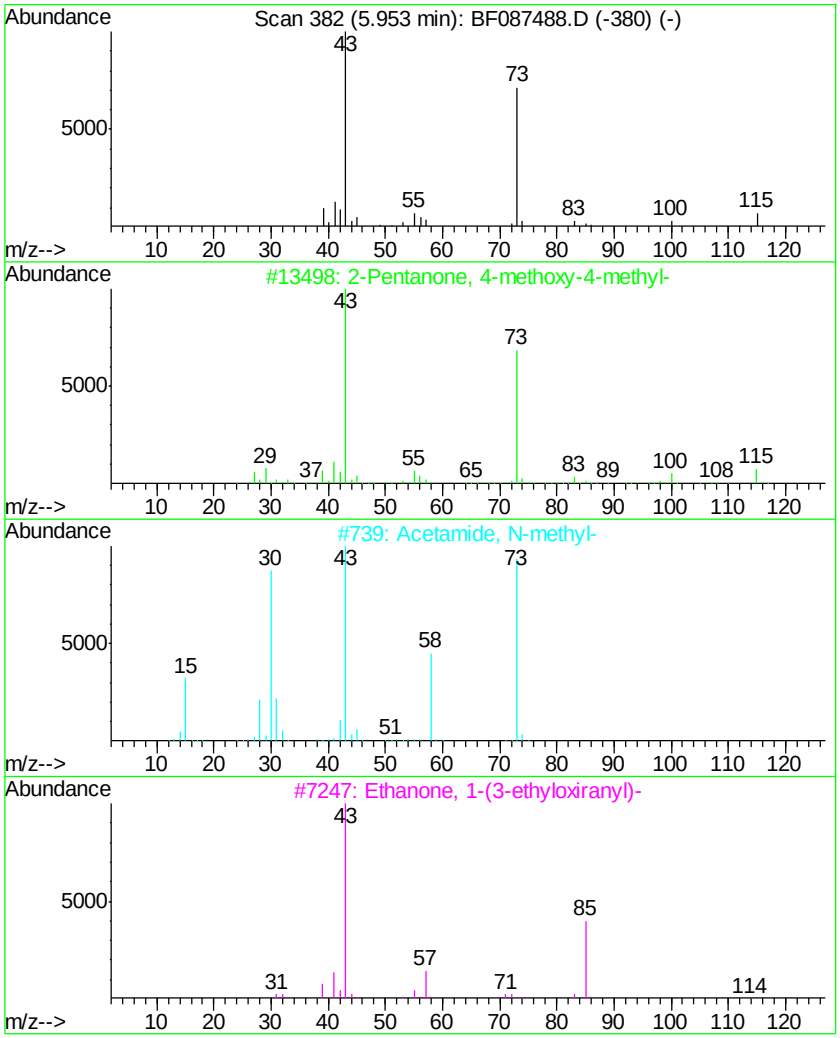
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

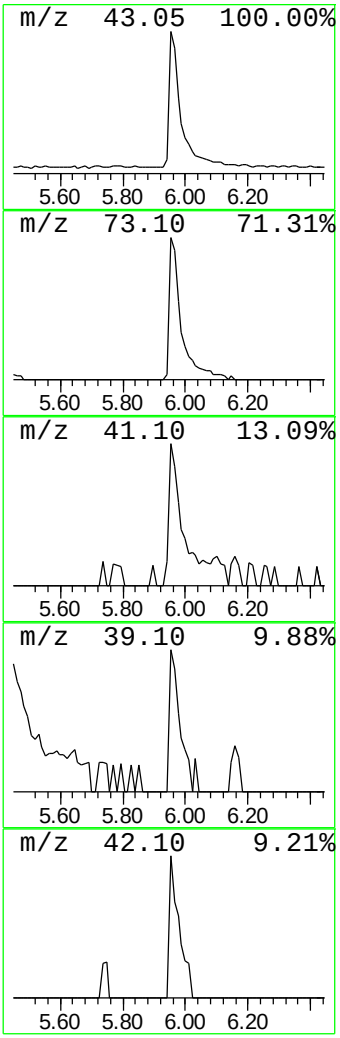
****

Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.95	2.51 ng	101429	1,4-Dichlorobenzene-d4	7.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	64
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	49
3	Ethanone, 1-(3-ethyloxiranyl)-	114	C6H10O2	017257-81-7	12
4	Pent-3-enylamine	85	C5H11N	087156-70-5	9
5	Butanal, 2-ethyl-	100	C6H12O	000097-96-1	9





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Sample : H3276-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

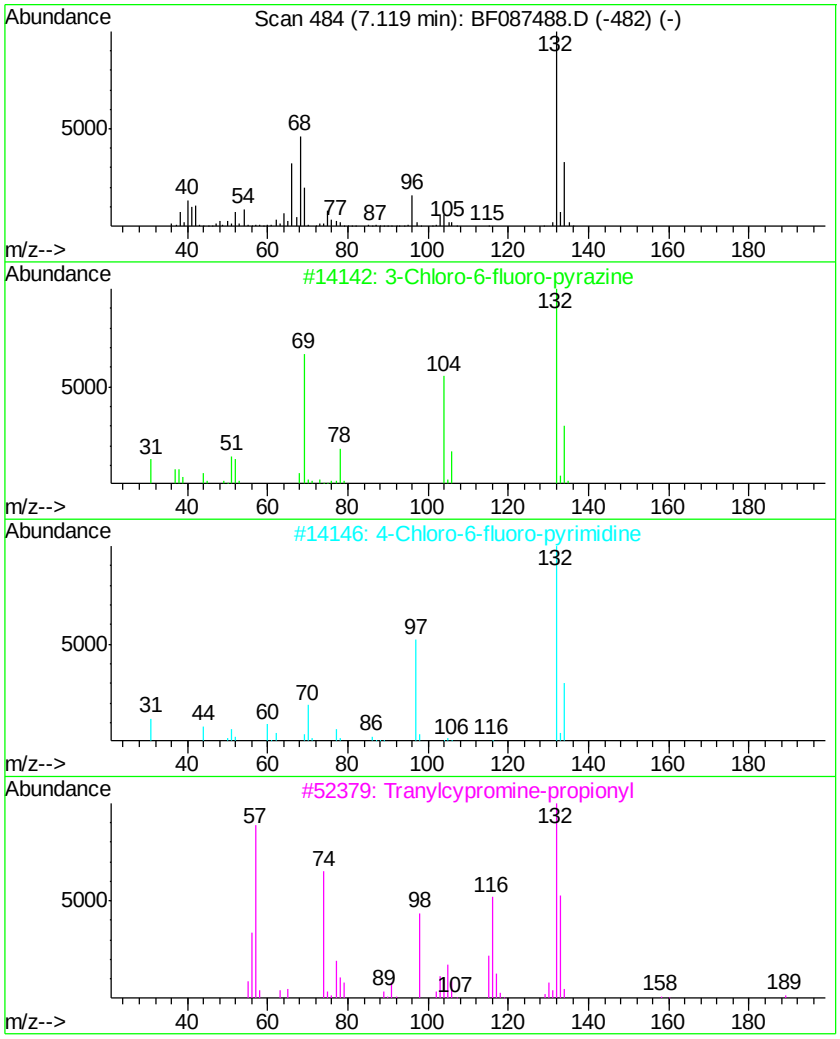
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

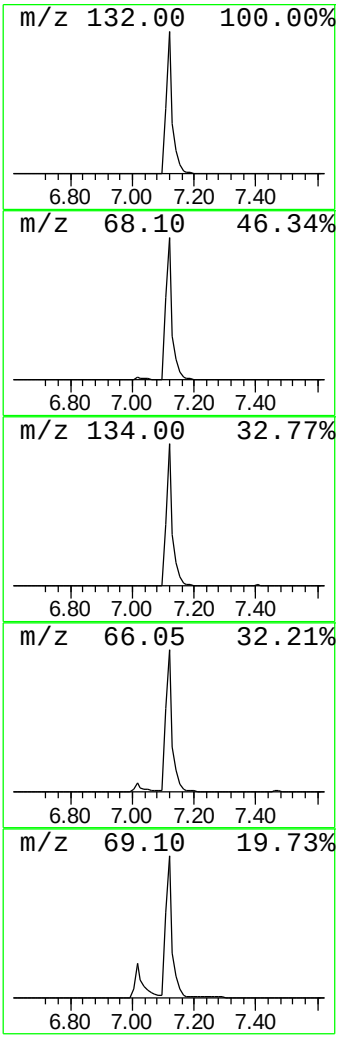
****

Peak Number 3 unknown7.12 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.12	80.50 ng	3253980	1,4-Dichlorobenzene-d4	7.46

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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : MW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

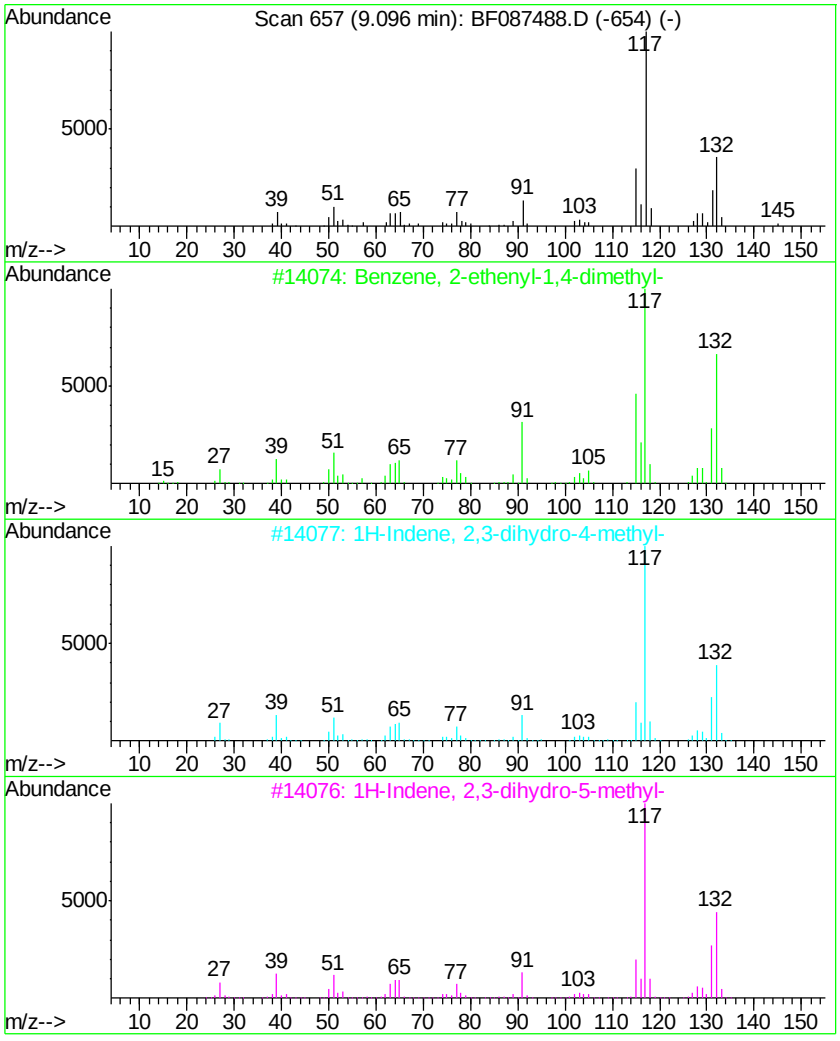
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

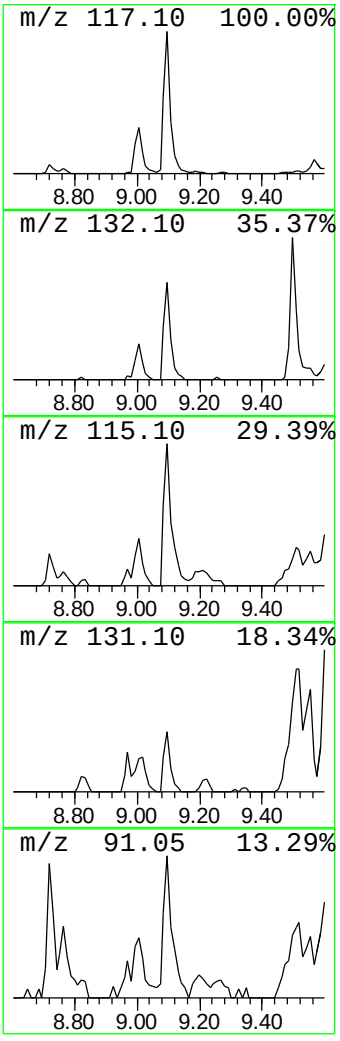
****

Peak Number 5 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.10	3.42 ng	196629	Naphthalene-d8	9.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	94
3	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	94
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	91
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	91





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ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

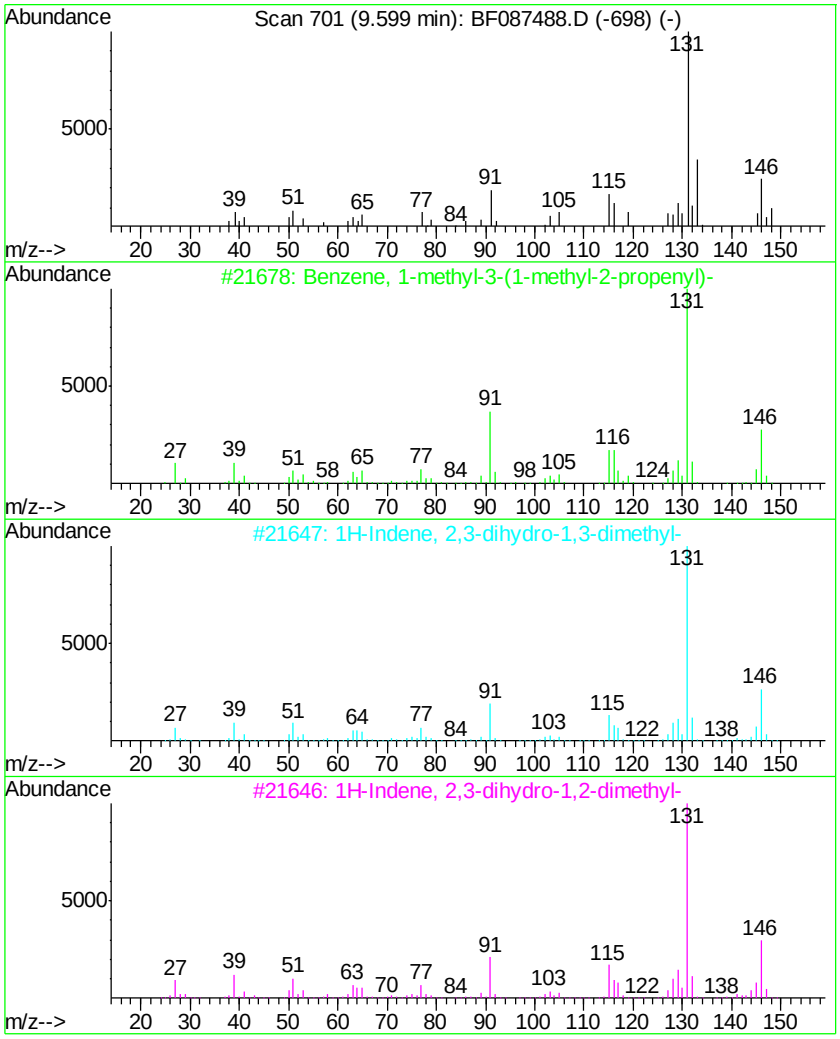
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

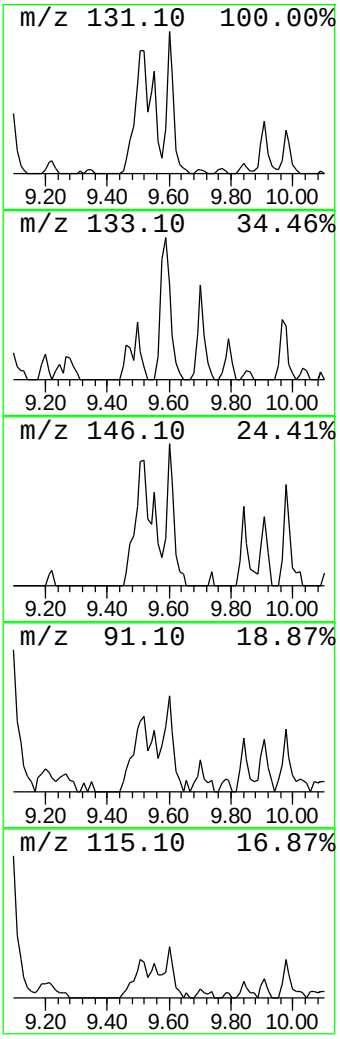
****

Peak Number 6 Benzene, 1-methyl-3-(1-meth... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.60	2.39 ng	137875	Naphthalene-d8	9.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-3-(1-methyl-2-...	146	C11H14	052161-57-6	89
2	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	81
3	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	81
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	146	C11H14	027087-54-3	81
5	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	81





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Sample : H3276-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

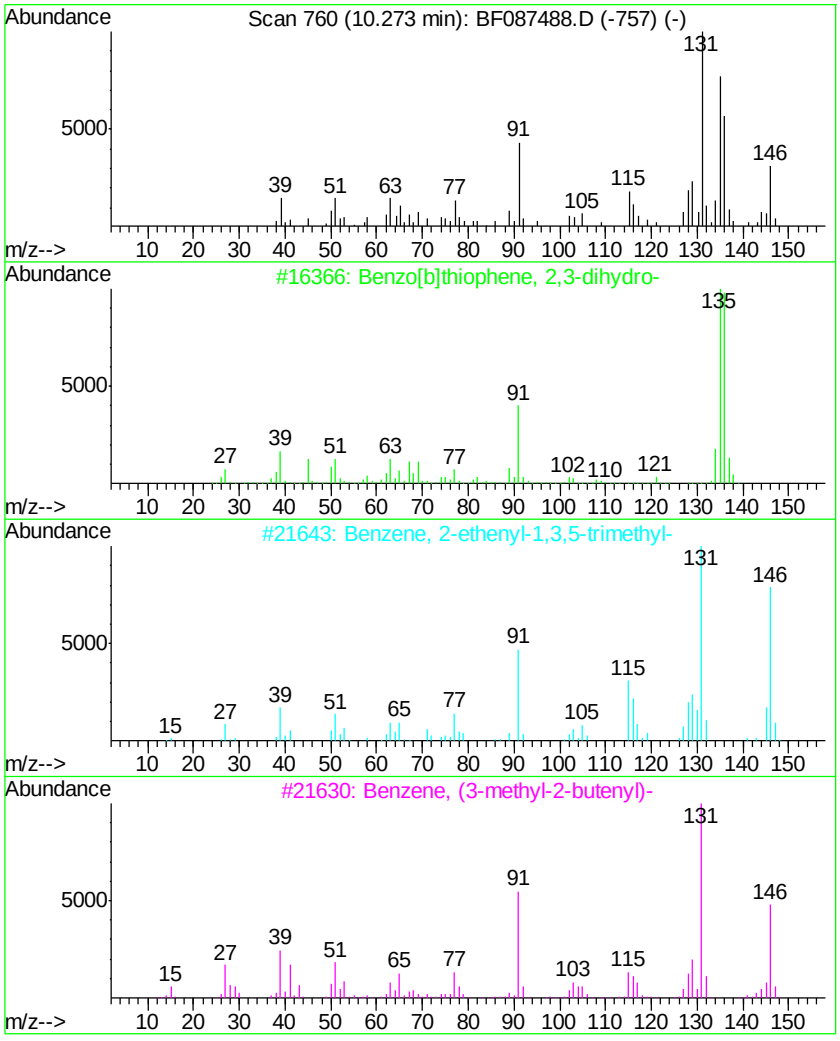
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

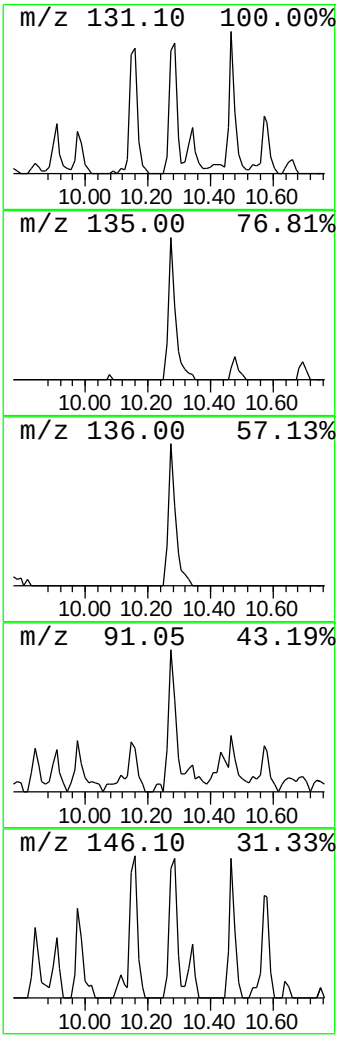
****

Peak Number 7 Benzo[b]thiophene, 2,3-dihy... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.27	2.47 ng	142250	Naphthalene-d8	9.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]thiophene, 2,3-dihydro-	136	C8H8S	004565-32-6	83
2	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	70
3	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	55
4	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	50
5	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	50





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Acq On : 28 May 2016 20:01
Operator : UM/SJ
Sample : H3276-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

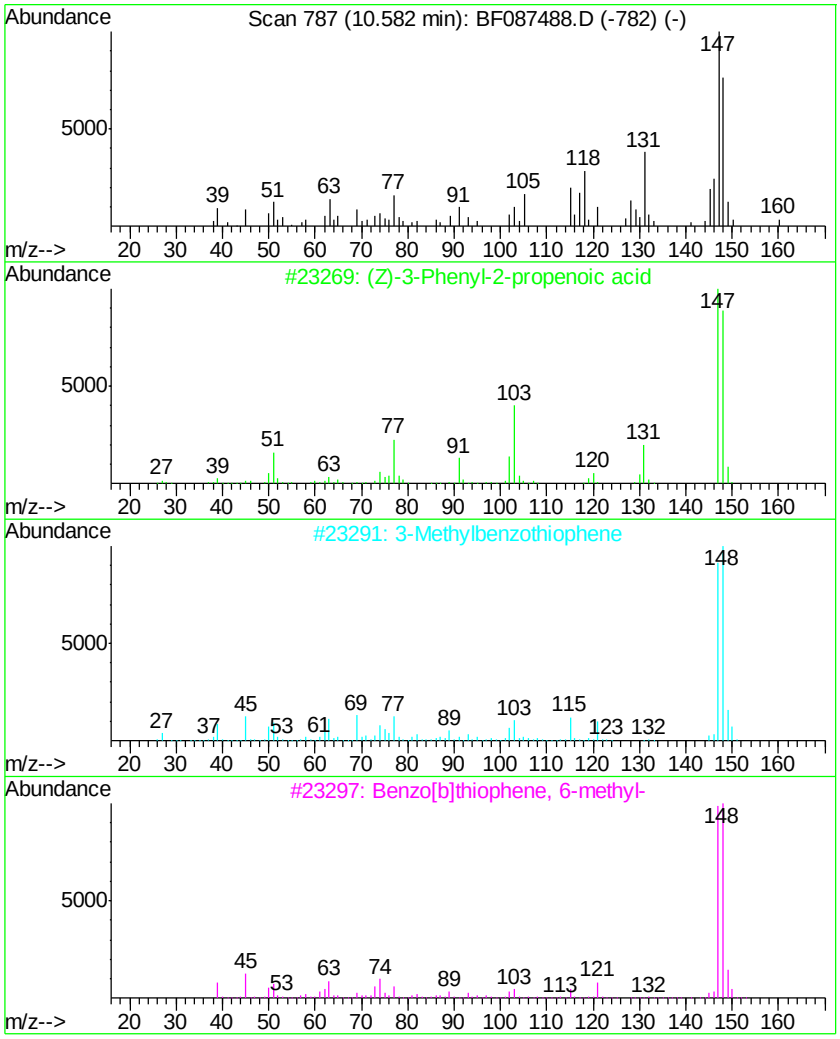
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

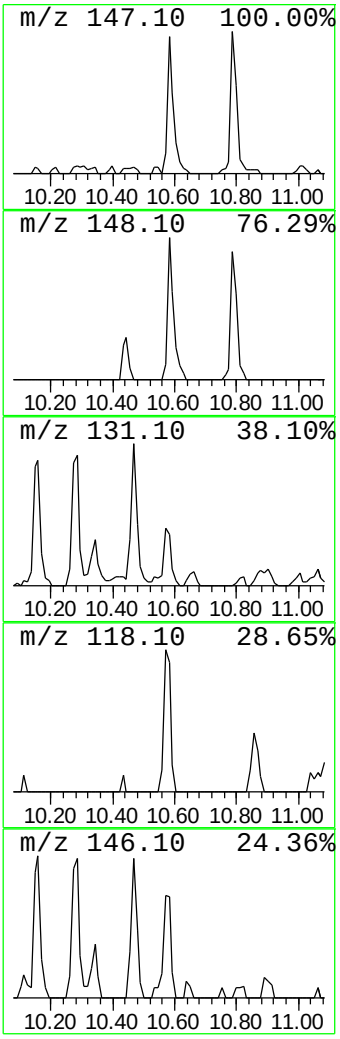
****

Peak Number 8 (Z)-3-Phenyl-2-propenoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.58	2.43 ng	139890	Naphthalene-d8	9.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-3-Phenyl-2-propenoic acid	148	C9H8O2	000102-94-3	60
2	3-Methylbenzothiophene	148	C9H8S	001455-18-1	60
3	Benzo[b]thiophene, 6-methyl-	148	C9H8S	016587-47-6	60
4	Benzo[b]thiophene, 5-methyl-	148	C9H8S	014315-14-1	53
5	Benzo[b]thiophene, 2-methyl-	148	C9H8S	001195-14-8	49





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052816\
Data File : BF087488.D
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Operator : UM/SJ
Sample : H3276-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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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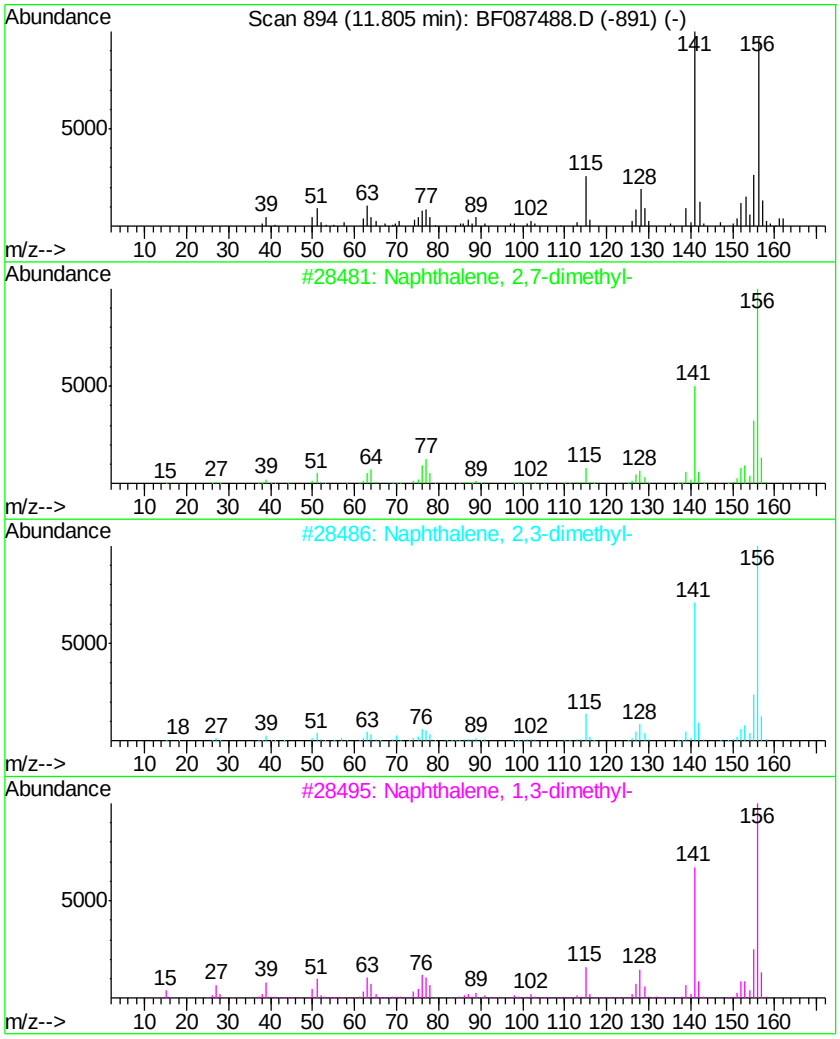
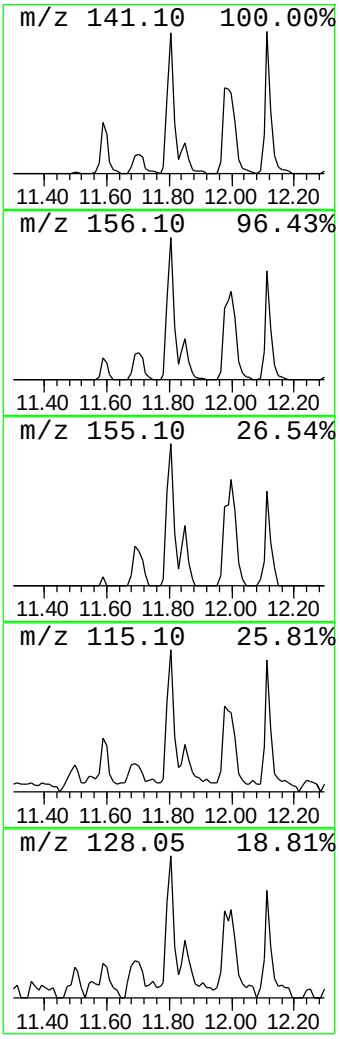
Peak Number 9 Naphthalene, 2,7-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.80	3.62 ng	213894	Acenaphthene-d10	12.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
2	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
3	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
4	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
5	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97





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Acq On : 28 May 2016 20:01
Operator : UM/SJ
Sample : H3276-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

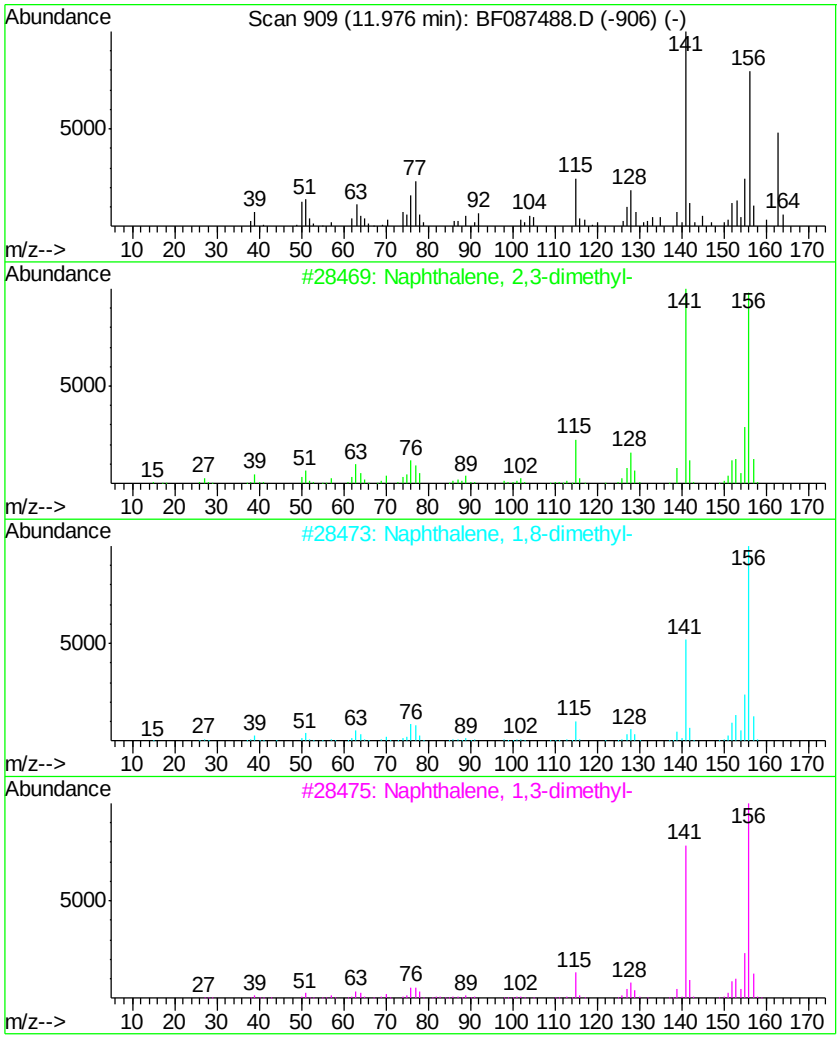
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

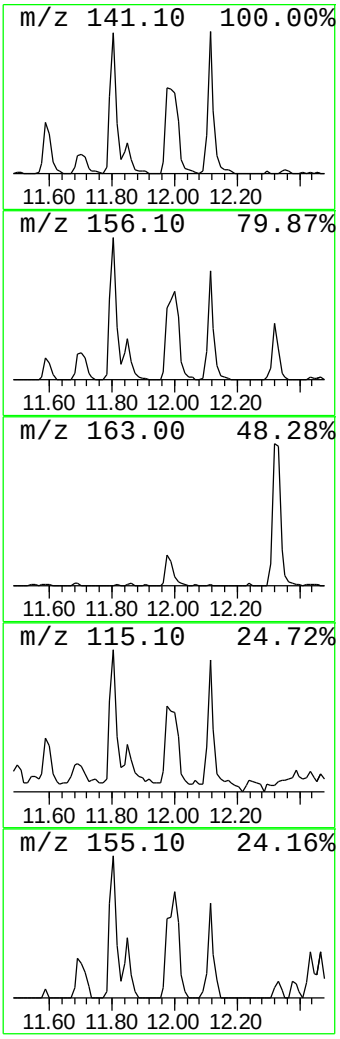
****

Peak Number 10 Naphthalene, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.98	4.67 ng	275845	Acenaphthene-d10	12.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	96
2	Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	96
3	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	95
4	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	95
5	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	95





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052816\
Data File : BF087488.D
Acq On : 28 May 2016 20:01
Operator : UM/SJ
Sample : H3276-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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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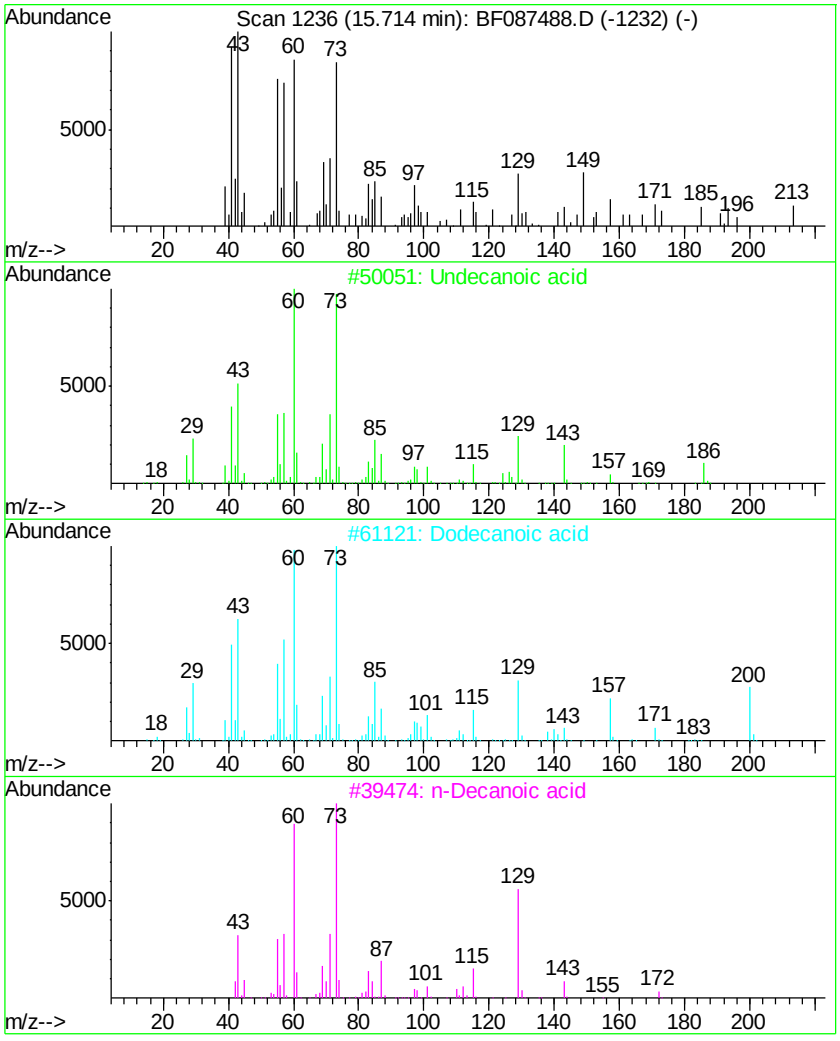
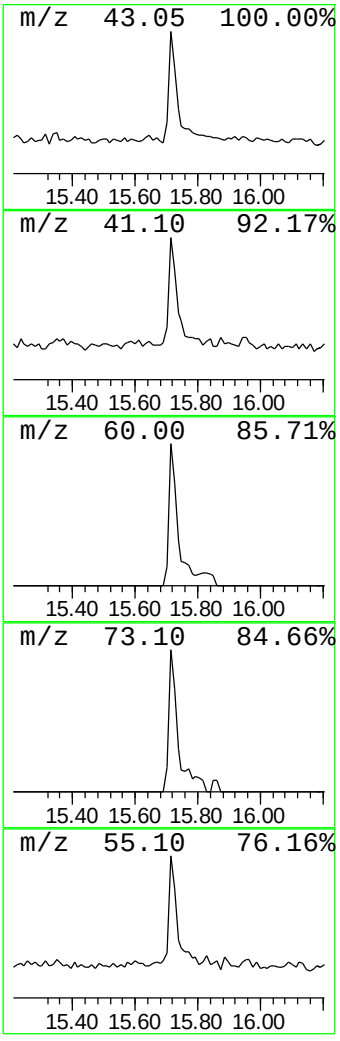
Peak Number 12 Undecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	2.07 ng	119436	Phenanthrene-d10	14.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	50
2	Dodecanoic acid	200	C12H24O2	000143-07-7	50
3	n-Decanoic acid	172	C10H20O2	000334-48-5	47
4	3-Ethylheptanoic acid	158	C9H18O2	014272-47-0	43
5	Trehalose	342	C12H22O11	000099-20-7	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052816\
Data File : BF087488.D
Acq On : 28 May 2016 20:01
Operator : UM/SJ
Sample : H3276-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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...	4.68	15.1	ng	609706	1	7.46	808409	20.0
2-Pentanone, 4-me...	5.95	2.5	ng	101429	1	7.46	808409	20.0
unknown7.12	7.12	80.5	ng	3253980	1	7.46	808409	20.0
Benzene, 2-etheny...	9.10	3.4	ng	196629	2	9.50	1151480	20.0
Benzene, 1-methyl...	9.60	2.4	ng	137875	2	9.50	1151480	20.0
Benzo[b]thiophene...	10.27	2.5	ng	142250	2	9.50	1151480	20.0
(Z)-3-Phenyl-2-pr...	10.58	2.4	ng	139890	2	9.50	1151480	20.0
Naphthalene, 2,7-...	11.80	3.6	ng	213894	3	12.32	1182060	20.0
Naphthalene, 2,3-...	11.98	4.7	ng	275845	3	12.32	1182060	20.0
Undecanoic acid	15.71	2.1	ng	119436	4	14.72	1153800	20.0